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# Applicability of the PROSPECT model for estimating protein and cellulose + lignin in fresh leaves

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ABSTRACT

Hyperspectral remote sensing of leaf biochemicals is critical for understanding many biochemical processes. Leaf biochemical contents (e.g., protein, cellulose and lignin) in fresh and dry leaves have been quantified from hyperspectral data using empirical models. However, they cannot be retrieved for fresh leaves by inverting radiative transfer models. We demonstrated the applicability of PROSPECT leaf optical properties model in the separation of specific absorption coefficients for protein and cellulose + lignin following a newly proposed algorithm, and evaluated the feasibility in estimating leaf protein and cellulose + lignin content through model inversion. Assessment was performed across a large variety of plant species benefiting from the Leaf Optical Properties Experiment (LOPEX) dataset. To alleviate ill-posed problems, inversion was performed over different spectral subsets. The PROSPECT model with newly calibrated specific absorption coefficients was able to accurately reconstruct leaf reflectance and transmittance. Leaf protein and cellulose + lignin were estimated at moderate to good accuracies for both fresh and dry leaves. The spectral subset of 2100–2300 nm yielded the most accurate estimation of leaf cellulose + lignin ($R^2 = 0.70$, RMSE = 5.21E−04 g/cm$^2$) and protein ($R^2 = 0.47$, RMSE = 2.75E−04 g/cm$^2$) in fresh leaves, which were comparable with those obtained from stepwise multiple linear regressions (protein: $R^2 = 0.83$, RMSE = 3.91E−04 g/cm$^2$; cellulose + lignin: $R^2 = 0.66$, RMSE = 2.02E−04 g/cm$^2$). Our results confirm the importance of selecting a proper spectral subset that contains sufficient information for a successful inversion. For the first time, we provide promising estimations of leaf protein in fresh leaves through inversion of a radiative transfer model, which can be applied at canopy level for regional mapping if coupled with a canopy reflectance model and air- or spaceborne hyperspectral imaging.



## 1. Introduction

Leaf protein, cellulose and lignin provide critical information about many biochemical processes, such as photosynthesis, respiration, and litter decomposition (Peterson & Hubbard, 1992). Proteins are the main nitrogen-containing biochemical constituent in plants (Kokaly, Asner, Ollinger, Martin & Wessman, 2009), and nitrogen is often a limiting factor for plant growth and important in terrestrial ecosystem carbon dynamics (Ollinger & Smith, 2005; Smith, Ollinger, Martin, Aber, Hallett & Goodale, 2002). Cellulose and lignin (hereafter referred to as "cellulose + lignin") is highly correlated with the total carbon in leaf (Jacquemoud, Ustin, Verdebout, Schmuck, Andreoli & Hosgood, 1996), and play a significant role in forest litter decomposition and nutrient cycling (Aber & Federer, 1992; Steudler, Bowden, Melillo & Aber, 1989). Therefore, remote estimation of leaf protein and cellulose + lignin is essential in producing an equivalent ratio of carbon/nitrogen (C/N), which will further improve the understanding of biogeochemical processes.

Two different techniques have been investigated for retrieving leaf protein and cellulose + lignin using hyperspectral data. Empirical methods have been the dominant techniques used to estimate the leaf parameters, focusing on building statistical regression models from the high correlations between their content and reflectance or its derivatives (Curran, 1989; Kokaly & Clark, 1999; Skidmore, Ferwerda, Mutanga, Van Wieren, Peel, Grant, et al., 2010; Zhao, Valle, Popescu, Zhang & Mallick, 2013). However, it proved difficult to transfer the empirical relationships across species or sites (LaCapra, Melack, Gastil & Valeriano, 1996; Martin & Aber, 1997). Moreover, the wavebands selected by statistical analysis from different studies have, on occasion, been inconsistent depending on using reflectance or transmittance, dry or fresh leaves, and have deviated from known absorption bands of leaf compounds (Curran, Dungan & Peterson, 2001; Huang, Turner, Dury, Wallis & Foley, 2004; Jacquemoud, Ustin, Verdebout, Schmuck, Andreoli & Hosgood, 1996).

Radiative transfer models (RTMs) describe the interaction of solar radiation in leaves based on laws of optics, thus offer advantages in

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**Table 1**
Statistics of the LOPEX dataset used in this study.

| Parameter | Unit | Min | Max | Mean | Std. |
|---|---|---|---|---|---|
| Equivalent water thickness (EWT) [a] | cm | 0.0046 | 0.0405 | 0.0114 | 0.0067 |
| Equivalent water thickness (EWT) [b] | cm | 1.85E−05 | 0.0009 | 0.0002 | 0.0001 |
| Protein | g/cm$^2$ | 2.92E−04 | 0.0020 | 0.0010 | 0.0003 |
| Cellulose + lignin | g/cm$^2$ | 1.47E−04 | 0.0046 | 0.0013 | 0.0010 |
| Leaf mass per area (LMA)[a] | g/cm$^2$ | 0.0019 | 0.0137 | 0.0053 | 0.0024 |
| Leaf mass per area (LMA) [b] | g/cm$^2$ | 0.0024 | 0.0165 | 0.0059 | 0.0026 |

[a] and [b] were for parameters in fresh and dry leaves, respectively.

robustness and transferability compared to empirical models (Darvishzadeh, Atzberger, Skidmore & Schlerf, 2011; Jacquemoud & Baret, 1990; Schlerf & Atzberger, 2006). RTMs have been widely applied to retrieve several leaf biochemical parameters (e.g., leaf chlorophyll, dry matter and water content) from remotely sensed data (Baret & Fourty, 1997a; Darvishzadeh, Skidmore, Schlerf & Atzberger, 2008; Feret, Francois, Asner, Gitelson, Martin, Bidel, et al., 2008; Omari, White, Staenz & King, 2013), but they have not been well developed for leaf protein and cellulose + lignin. Several studies (Fourty, Baret, Jacquemoud, Schmuck & Verdebout, 1996; Jacquemoud, Ustin, Verdebout, Schmuck, Andreoli & Hosgood, 1996) attempted to incorporate leaf protein, cellulose + lignin into the absorption and scattering processes in radiative transfer models, such as the PROSPECT leaf optical properties model (Jacquemoud & Baret, 1990). Leaf protein and cellulose + lignin for dry leaves could be moderately well estimated ($R^2$ = 0.49–0.84) through PROSPECT model inversion (Fourty, Baret, Jacquemoud, Schmuck & Verdebout, 1996; Jacquemoud, Ustin, Verdebout, Schmuck, Andreoli & Hosgood, 1996), but so far, these parameters have not been successfully estimated for fresh leaves using the PROSPECT model (Botha, Zebarth & Leblon, 2006; Jacquemoud, Ustin, Verdebout, Schmuck, Andreoli & Hosgood, 1996; Kokaly, Asner, Ollinger, Martin & Wessman, 2009). On fresh leaves, leaf reflectance and transmittance are insensitive to protein because of its small percentage in the leaf mass (Baret & Fourty, 1997b; Jacquemoud, Ustin, Verdebout, Schmuck, Andreoli & Hosgood, 1996). Moreover, the high covariance with water and other nitrogen-containing compounds, such as chlorophyll, has led to inconsistencies in retrieving leaf protein via PROSPECT inversion (Jacquemoud & Baret, 1990; Jacquemoud, Ustin, Verdebout, Schmuck, Andreoli & Hosgood, 1996; Kokaly, Asner, Ollinger, Martin & Wessman, 2009). The idea of incorporating leaf protein, and cellulose + lignin into the PROSPECT model was therefore abandoned in the 1990s (Jacquemoud & Baret, 1990; Jacquemoud, Ustin, Verdebout, Schmuck, Andreoli & Hosgood, 1996), and they were represented by a more general parameter of "dry matter content" (Fourty, Baret, Jacquemoud, Schmuck & Verdebout, 1996).

The retrieval of leaf parameters (e.g. protein and cellulose + lignin) in fresh leaves by inversion of PROSPECT remains challenging. The first issue needed to be resolved is the determination of specific absorption coefficients of leaf biochemicals, which describes the absorption property of a leaf, together with the content of these biochemicals (Jacquemoud & Baret, 1990). The specific absorption coefficients are considered to be inherent properties, which are constant across samples and species (Feret, Francois, Asner, Gitelson, Martin, Bidel, et al., 2008). It is difficult to determine these coefficients for the model; the coefficient for pure liquid water and chlorophyll has been well investigated (Buiteveld, Hakvoort & Donze, 1994; Kou, Labrie & Chylek, 1993; Wieliczka, Weng & Querry, 1989), but gaps still exists for leaf pigments (i.e. chlorophyll a and b) and other cell wall constituents (i.e. protein, cellulose + lignin) (Feret, Francois, Asner, Gitelson, Martin, Bidel, et al., 2008). The obstacles lie in measuring the coefficients in vivo, as well as extracting each biochemical constituent for its measurement in vitro (Porra, 2002). Therefore, the in vivo specific absorption coefficients are normally calibrated from intact leaves via model inversion using the measured spectra and biochemical contents (Feret, Francois, Asner, Gitelson, Martin, Bidel, et al., 2008; Fourty, Baret, Jacquemoud, Schmuck & Verdebout, 1996; Jacquemoud & Baret, 1990; Jacquemoud, Ustin, Verdebout, Schmuck, Andreoli & Hosgood, 1996).

The "ill-posed" inverse problem of radiative transfer model is the second challenge in the retrieval of leaf protein and cellulose + lignin. Different combinations of leaf parameters can generate similar leaf spectra. And the leaf parameters which make greater contribution to leaf reflectance, such as leaf structure parameter and leaf water, bring more uncertainties in the retrieval of protein and cellulose + lignin. Several studies have demonstrated that selecting spectral subsets will return a higher accuracy than using full wavelengths in inverting radiative transfer models (Darvishzadeh, Skidmore, Schlerf & Atzberger, 2008; Meroni, Colombo & Panigada, 2004; Schlerf & Atzberger, 2006). The reasons for this can be poorly measured spectra, some wavelengths may not be well described in the model (Schlerf & Atzberger, 2006), or extra bands may add noise without adding significant information (Weiss, Baret, Myneni, Pragnère & Knyazikhin, 2000). In addition, higher accuracies could be obtained for estimating leaf parameters if the inversion approach would consider a specific merit function assigned for each parameter and incorporate sensitive spectral bands determined by sensitivity analysis (Li & Wang, 2011; Zhao, Guo, Huang, Reddy, Lee, Fletcher, et al., 2014).

The radiative transfer model PROSPECT has been recalibrated with a newly proposed algorithm which can simulate leaf optical properties with a higher accuracy than previous versions (Feret, Francois, Asner, Gitelson, Martin, Bidel, et al., 2008). In their study, the incidence angle of incoming radiation was reassessed, and the specific absorption coefficients of leaf constituents and the refractive index were recalibrated for two new version models (PROSPECT-4 and PROSPECT-5). PROSPECT-5 is the same as PROSPECT-4 except the separation of total chlorophylls and total carotenoids in the visible range of 400–750 nm. The algorithm has been tested for accurate simulation of leaf reflectance (Li & Wang, 2011; Ma, Chen, Wang, Li & Jiapaerl, 2012), and has been further adapted to incorporate tannin as an input parameter for assessing the quality of tea in Tea-PROSPECT (Bian, 2013). However, to our knowledge, the newly proposed algorithm has not been evaluated for determining the specific absorption coefficients for leaf constituents, such as protein, cellulose, hemicellulose, and lignin. And the potential of PROSPECT-5 for retrieving leaf constituents through model inversion needs to be further explored.

The estimation of leaf constituents (e.g. protein and cellulose + lignin) using fresh leaf spectra through the radiative transfer model PROSPECT has not been studied extensively (Botha, Zebarth & Leblon, 2006; Jacquemoud, Ustin, Verdebout, Schmuck, Andreoli & Hosgood, 1996), probably because of the notion that there may be little sensitivity of leaf optical properties to the leaf constituents. The aim of our study was therefore to evaluate the most recent PROSPECT model (version 5) for estimating leaf protein, cellulose + lignin by recalibrating their specific absorption coefficients, using the calibration algorithm proposed by Feret, Francois, Asner, Gitelson, Martin, Bidel, et al. (2008). Our specific objectives were: (1) to test if the specific absorption coefficients could be robustly estimated across species from a model calibration procedure; (2) to test if the PROSPECT model with the recalibrated coefficients could successfully simulate leaf reflectance

**Table 2**
Ranges of the input parameters used in the recalibrated PROSPECT-5 model.

| Parameter | Unit | Min | Max |
|---|---|---|---|
| Leaf structure parameter ($N$) | – | 1 | 3 |
| Equivalent water thickness (EWT) [a] | cm | 0.001 | 0.05 |
| Equivalent water thickness (EWT) [b] | cm | 0.00001 | 0.001 |
| Protein | g/cm$^2$ | 0.0001 | 0.002 |
| Cellulose + lignin | g/cm$^2$ | 0.0001 | 0.005 |

[a] and [b] were for parameters in fresh and dry leaves, respectively.