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Needle chlorophyll content estimation through model inversion using hyperspectral data from boreal conifer forest canopies

Pablo J. Zarco-Tejada[a,*], John R. Miller[a,b], John Harron[a,1], Baoxin Hu[b,c], Thomas L. Noland[d], Narendra Goel[e], Gina H. Mohammed[d,2], Paul Sampson[d]

[a] Centre for Research in Earth and Space Science (CRESS), York University, 4700 Keele Street, Toronto, Canada M3J 1P3
[b] Department of Physics and Astronomy, York University, Toronto, Canada M3J 1P3
[c] Canadian Space Agency, 6767 Route De L'Aeroport Saint-Hubert, Québec, Canada J3Y 8Y9
[d] Ontario Forest Research Institute, Ontario Ministry of Natural Resources, Sault Ste. Marie, Ontario, Canada P6A 2E5
[e] Department of Computer Science,Wayne State University, Detroit, MI 48202, USA

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Abstract

Leaf chlorophyll content in coniferous forest canopies, a measure of stand condition, is the target of studies and models linking leaf reflectance and transmittance and canopy hyperspectral reflectance imagery. The viability of estimation of needle chlorophyll content from airborne hyperspectral optical data through inversion of linked leaf level and canopy level radiative transfer models is discussed in this paper. This study is focused on five sites of Jack Pine (*Pinus banksiana* Lamb.) in the Algoma Region (Canada), where field, laboratory and airborne data were collected in 1998 and 1999 campaigns. Airborne hyperspectral CASI data of 72 bands in the visible and near-infrared region and 2 m spatial resolution were collected from 20 × 20 m study sites of Jack Pine in 2 consecutive years. It was found that needle chlorophyll content could be estimated at the leaf level ($r^2 = 0.4$) by inversion of the PROSPECT leaf model from needle reflectance and transmittance spectra collected with a special needle carrier apparatus coupled to the Li-Cor 1800 integrating sphere. The Jack Pine forest stands used for this study with LAI > 2, and the high spatial resolution hyperspectral reflectance collected, allowed the use of the SPRINT canopy reflectance model coupled to PROSPECT for needle chlorophyll content estimation by model inversion. The optical index R750/R710 was used as the merit function in the numerical inversion to minimize the effect of shadows and LAI variation in the mean canopy reflectance from the 20 × 20 m plots. Estimates of needle pigment content from airborne hyperspectral reflectance using this linked leaf-canopy model inversion methodology showed an $r^2 = 0.4$ and RMSE = 8.1 μg/cm^2 when targeting sunlit crown pixels in Jack Pine sites with pigment content ranging between 26.8 and 56.8 μg/cm^2 (1570–3320 μg/g).

Keywords: Chlorophyll; Canopy modelling; Needle reflectance; Hyperspectral; Optical indices; Radiative transfer

1. Introduction

The literature conclusively records that pigment content can be statistically linked with reflectance data at the leaf and canopy levels. This relationship is primarily through reflectance ratio indices, spectral derivatives and spectral position, particularly in the red edge spectral region. At the leaf level, there has been an emphasis on the identification of optical indices for optimum pigment correlation (e.g. Carter, 1994), for the study of the species and seasonal dependence (e.g. Belanger, Miller, & Boyer, 1995), and for correlation with bioindicators of leaf status or vigour (e.g. Luther & Carroll, 1999; Zarco-Tejada, Miller, Mohammed, Noland, & Sampson, 1999). Such relationships have been explored at the canopy level through data from field spectrometers and airborne imaging spectrometers, as well as documenting and exploring the potentially confounding effects of canopy structure variables, as leaf area index (Rock, Hoshizaki, & Miller, 1988; Gong, Pu, & Miller, 1992; Matson, Johnson, Billow, Miller, & Pu, 1994; Gong,

* Corresponding author. Present Address: Center for Spatial Technologies and Remote Sensing (CSTARS), Department of Land, Air, and Water Resources (LAWR), Veihmeyer Hall, University of California, Davis, CA 95616-8671, USA.
E-mail addresses: pzarco@ucdavis.edu (P.J. Zarco-Tejada), jrmiller@yorku.ca (J.R. Miller).
[1] Present Address: Spectral Applied Research Inc., 10 North Rivermede Rd. Concord, Ontario, Canada L4K 2H2.
[2] Present Address: P&M Technologies, 66 Millwood St., Sault Ste. Marie, Ontario, Canada P6A 6S7.

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Pu, & Miller, 1995; Curran, Kupiec, & Smith, 1997; Shaw, Malthus, & Kupiec, 1998; Zarco-Tejada et al., 1999; Lucas, Curran, Plummer, & Danson, 2000).

Considerable progress has been reported recently in the development of suitable methods for broad leaf canopies to link leaf optical properties with canopy structural characteristics through radiative transfer modelling. At the leaf level, the PROSPECT model (Jacquemoud & Baret, 1990) has seen widespread validation and use for estimation of leaf biochemical constituents by inversion of measured reflectance and transmittance data (Jacquemoud, Ustin, Verdebout, Schmuck, Andreoli, & Hosgood, 1996; Kuusk, 1998; Demarez & Gastellu-Etchegorry, 2000; Zarco-Tejada, Miller, Noland, Mohammed, & Sampson, 2001). Research in which PROSPECT has been linked to the SAIL canopy reflectance model (Verhoef, 1984), or to SAILH in which the hotspot effect (Kuusk, 1985) is incorporated, have added significantly to the understanding of relationships between leaf biochemistry, canopy structural parameters, and above-canopy bi-directional reflectance. Numerical inversions of these coupled models have been reported (Jacquemoud, 1993; Jacquemoud, Baret, Andrieu, Danson, & Jaggard, 1995; Kuusk, 1998; Demarez & Gastellu-Etchegorry, 2000; Jacquemoud, Bacour, Poilve, & Frangi, 2000) to allow airborne above canopy reflectance to simultaneously infer leaf level pigment content and LAI in crop canopies for a given set of viewing geometry conditions. Another recent example of simulations with a coupled leaf and dense canopy models is the work of Ganapol, Johnson, Hlavka, Peterson, and Bond (1999).

Forest canopies, however, cannot be treated simply as a turbid medium such as for crop canopies. This restriction is due to the above-canopy radiometric texture arising from crown shadowing in closed canopies and the increasing dominance of effects due to background and shadows with open canopies. Recently, several 3-D canopy models (Myneni, Marshak, Knyazikhin, & Asrar, 1991; Li, Strahler, & Woodcock, 1995; North 1996; Gastellu-Etchegorry, Demarez, Pinel, & Zagolski, 1996; Goel & Thompson, 2000) have allowed the simulation of the relationship between optical indices and leaf pigment content coupled with the interplay of forest structure. Demarez and Gastellu-Etchegorry (2000) provide a detailed modelling study of the relationship between leaf pigment and canopy red edge position linking PROSPECT and DART. The important confounding effects of understory reflectance and canopy structural parameters in deciduous forest canopies are described.

A recent study using CASI hyperspectral reflectance data from 12 Sugar Maple (*Acer saccharum* M.) forest sites with dense closed canopies (LAI > 4) demonstrated the feasibility of radiative transfer methods for pigment estimation (Zarco-Tejada et al., 2001). Chlorophyll $a+b$ (chl_{a+b}) estimation by scaling up and radiative transfer model inversion techniques were shown to be feasible, with root mean square errors from 3 to 5.5 μg/cm^2 for a range in leaf chlorophyll between 19.1 and 45.8 μg/cm^2. Analysis involved scaling-up and numerical inversion methods using PROSPECT coupled to the SAILH radiative transfer model studying the effect of different techniques and merit function design in the parameter estimation by model inversion. Comparison of model-estimated reflectance with sensor-measured reflectance by iterative optimization techniques to estimate input model parameters requires building a merit function (error) which needs to be minimized. The study of the merit function in the numerical inversion showed that red edge optical indices used in the minimizing function perform better than when all single spectral reflectance channels from hyperspectral airborne CASI data were used. It was also demonstrated that merit functions built with red edge spectral transforms such as R750/R710 (Zarco-Tejada et al., 2001) minimize the forest canopy structure, shadows and openings, reducing the effects due to LAI variation.

One of the goals of BOREAS was to stimulate the development of radiative transfer modelling suited to conifer boreal forests. BOREAS data sets have been instrumental in the validation of DART (Gastellu-Etchegorry et al., 1996), 4-Scale (Chen & LeBlanc, 1997), GORT (Li et al., 1995) and flavours of Monte Carlo models (North, 1996; Goel & Thompson, 2000 [SPRINT]). Moreover, BOREAS leaf optical properties (Middleton, Chan, Rusin, & Mitchell, 1997; Middleton, Walter-Shea, Mesarch, Chan, & Rusin, 1997) and understory reflectance measurements (Miller, White, Chen, McDermid, Peddle, Fournier, Shepherd, Rubinstein, Freemantle, Soffer, & LeDrew, 1997) have served as essential model parameterizations to these evaluations. With the introduction of the needle model LIBERTY (Dawson, Curran, & Plummer, 1998), simulations with coupled leaf and canopy models for conifer forest stands have begun to provide new insights into the factors affecting biophysical parameter retrieval in boreal conifer forests (Dawson, Curran, North, & Plummer, 1997). The aim of this paper is to further contribute to this understanding for boreal coniferous canopies, investigating physical methods and radiative transfer assumptions for estimation of pigment content from hyperspectral data.

This paper reports on the results of a study to explore the extendibility to coniferous forests of the approach described by Zarco-Tejada et al. (2001) for the retrieval of leaf pigment content in sugar maple closed-canopy stands. This study involves CASI hyperspectral data from 2 successive years from five Jack Pine sites in the Algoma region (Canada). Airborne imagery was complemented by needle level measurements of pigment content and reflectance and transmittance. Optical measurements of needles were carried out with a specially designed apparatus, calibrated and tested with BOREAS Jack Pine data, resulting in improvements in needle-level reflectance and transmittance measurements. The implications for these revisions in needle optical properties on pigment retrieval at the needle level are presented, followed by model inversions tested with a set of coniferous sites from the boreal region. The PROSPECT model was used for the leaf level simulations, linked to SPRINT for the modelling at the canopy level. Details of these approaches and results are described below.

2. Experimental methods and data sets

2.1. Study sites

Five Jack Pine (*Pinus banksiana* Lamb.) stands from the Algoma region of northwestern Ontario, Canada were selected as the study sites (Fig. 1). Sampling was carried out in late July of 1998 and 1999, collecting samples from the top of the crowns at each of the 20 × 20 m study sites. Five trees per study site were selected, sampling one branch from each tree, and selecting four shoots per branch for tissue measurement of chl_{a+b} and spectral measurements of reflectance and transmittance. Measurements of stand parameters as well as shoot and needle parameters, summarized in Table 1 were essential to characterize the canopy architecture for the modelling aspect of this study.

2.2. Leaf sampling and pigment measurements

Chlorophyll *a* and *b* and total carotenoid measurements were carried out for Jack Pine needles. Branches collected from the tops of crowns were placed in a cooler with ice (0 °C) for transport to the laboratory and stored at − 23 °C immediately after arrival.

For the 1998 field study, each branch sample was used to provide eight shoots, four for biochemical analysis and four for optical leaf measurements. The emphasis in this sampling was to produce mean biochemical and optical results for each stand by averaging the results from the five trees per study plot. In 1999, the objective of sampling was broadened to also allow biochemical analysis results from specific shoots to be correlated with optical measurements from specific needles selected from the same shoot. As the field campaigns were carried out in late July, no effort was made to separately sample 1st year and 2nd year needles.

One gram fresh weight of needles from each selected shoot was ground with a mortar and pestle with liquid N_2 and then 0.2 g placed in a 15 ml. centrifuge tube for pigment extraction and 0.8 × *g* placed in container for dry weight determination. Dry weight was determined by oven drying at 80 °C for 24 h, and re-weighing. Chlorophyll $a+b$ and total carotenoids concentrations were determined by adding 10 ml of *N*,*N*-dimethylformamide (Spectralanalyzed grade, Fisher Scientific, Tustin, CA) to the 15 ml. tube. Tubes were placed horizontally in a darkened 4 °C orbital shaker set to 100 rpm for two h to extract pigments, centrifuged at 5 °C and 5,000 g for 20 min, and placed in a dark, 4 °C refrigerator for 20 min. Absorbance measured at 663.8 nm, 646.8 nm and 480 nm with a Cary one spectrophotometer enabled chlorophyll *a*, chlorophyll *b* and total carotenoid concentrations calculation using the extinction coefficients derived by Wellburn (1994). Mean, maximum and minimum chlorophyll concentrations observed for Jack Pine measurements are reported in Table 1.

2.3. Needle optical properties measurement method

Accurate measurements of leaf optical properties are critical to the development and validation of a leaf model. Reflectance and transmittance spectra modelled at the leaf level for a given amount of biochemical constituents are essential for the successful link with a forest canopy model. The model inversion successes using PROSPECT summarized previously for broad leaf species is evidence of this critical step. Whereas a methodology using the Li-Cor 1800 integrating sphere (Li-Cor, Lincoln, NE, USA) is widely used for accurate measurements of the reflectance and transmittance spectra of leaves of broad leaf species, reliable estimates for conifer needles has remained a difficult challenge.

A methodology introduced by Daughtry, Biehl, and Ranson, (1989) for conifers (*Daughtry's method*) was adapted to the Li-Cor 1800 in which needle samples are presented to the integrating sphere port with a regular spacing between them, since the irregular shape of needles makes inter-needle gaps unavoidable. The most significant challenge in this approach is the very accurate measurements needed of the radiant flux between the needles so that the radiant flux interacting with the needles can be accurately inferred. Subsequently, Middleton, Chan, et al. (1997), Middleton, Walter, et al. (1997) introduced a revised measurement protocol designed to improve the accuracy of the gap effect estimation. Significantly for this study, based on this revised methodology, Middleton, Chan, et al. (1997) report Jack Pine needle reflectance and transmittance spectra for both the adaxial and abaxial surfaces during the BOREAS project.

A new methodology was introduced during the BOREAS project by Harron and Miller (1995) for the measurement of needle optical properties (*Harron's method*). Comparisons of reflectance and transmittance measurements made with the *Daughtry's method* and the *Harron's method* on needle samples acquired at BOREAS have now been completed in Harron (2000). The detailed presentation of the method and equations described in Harron (2000) are beyond the scope of this paper and will be presented in a forthcoming publication. Since *Harron's method* has been used for optical measurements of needles used in this study, a brief description of basis of the method follows.

In order to measure the reflectance and transmittance of small area samples such as conifer needles, an efficient method of presenting the samples to the integrating sphere is needed. Using a carrier in which the needles are mounted is a logical choice and leads to the task of how to make an accurate measurement of the reflectance or transmittance of the sample while minimizing the effect of the needle carrier. For this design, a radiometric model of the integrating sphere with a compound target was developed. Expressions were developed using this model for calculating the reflectance and transmittance of samples which are smaller than the sample port held in place with a carrier (Harron, 2000).

The carrier-based measurement method (*Harron's method*) and the *Daughtry's method* both use reflectance characteristics and areas of the sphere as correction terms in the calculation of the actual transmittance and reflectance of the samples. In the *Daughtry's method*, a careful measurement of the gap fraction between the needles in the port is key. More importantly, the method fails to consider specular scattered light from the curved needle surface which escapes from the sphere in the reflectance measurements,

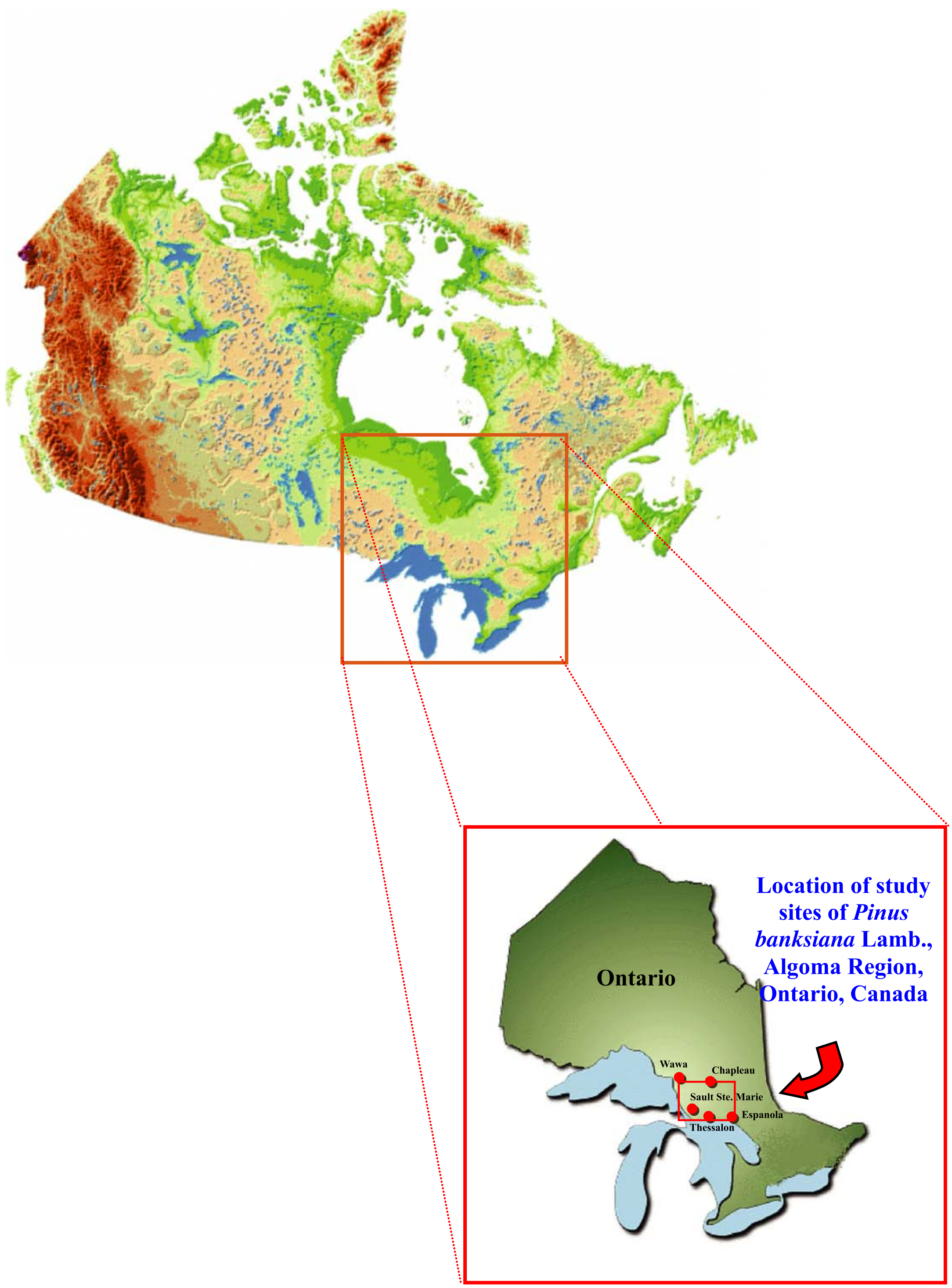

Fig. 1. Location of the study sites of *Pinus banksiana* Lamb. used in this research work, selected from existing provincial plot networks in the Algoma Region (Ontario, Canada), Sault Ste. Marie District, representing a range of productivity and decline.

Table 1
Nominal values and range of parameters used for leaf and canopy modelling with PROSPECT and SPRINT for Jack Pine study sites

Canopy structural parameters	Nominal Values
Tree density	1100/ha
Distribution of trees	Poisson distribution
Crown shape	Irregular conical (assumed ellipsoidal)
Height of trunk	8.5 m
Height of tree	15.0 m
Trunk radius	8.3 cm
Crown radius	2.0 m
Leaf angle distribution	Assumed spherical
Shoot area	0.0008 m^2
Canopy effective LAI	2.5
Leaf area density	0.4171 /m
Leaf and shoot structural parameters	Nominal values and range
Leaf thickness	0.062 cm (0.057–0.076)
Specific Leaf Area (fresh leaves)	20.9 cm^2/g (17.9–23.7)
Specific Leaf Area (dry weight) SLA	48.1 cm^2/g (37.7–58.6)
Leaf biochemical parameters	Range of values
Chlorophyll *a*	1037–2715 $\mu g \cdot g^{-1}$
Chlorophyll *b*	274–997 $\mu g \cdot g^{-1}$
Chlorophyll *a*+*b*	1286–3588 $\mu g \cdot g^{-1}$
Carotenoids	243–611 $\mu g \cdot g^{-1}$
Water (% of dry mass)	97.3–179.3

Canopy structural parameters were used in the SPRINT model for simulation of the canopy reflectance by radiative transfer. Leaf and shoot structural parameters, and leaf biochemical parameters were used for needle-level simulation of reflectance and transmittance using the PROSPECT radiative transfer model.

and which is introduced into the sphere in the transmittance measurements. Using the carrier-based method, the effect of this specular scattered light is eliminated completely. As a consequence, the difference between the needle optical properties measured by the two methods is approximately an offset (Harron, 2000) which affects the estimation of biochemical constituents using radiative transfer model inversion techniques.

Five needles from a sample shoot were needed for each reflectance and transmittance measurement carried out using the *Harron's method*. Each needle was measured for thickness and mounted in the specially designed black anodized carrier. Needle reflectance and transmittance measurements were acquired using the carrier-based method, which employed a Li-Cor 1800-12 Integrating Sphere. The apparatus was coupled by a 200-μm diameter single mode fibre to an Ocean Optics model ST 1000 spectrometer (Ocean Optics, Dunedin, Fl. USA) with a 1024 element detector array, yielding a 0.5 nm sampling interval and ~ 7.3 nm spectral resolution in the 340–860 nm range. Software was designed to allow detailed control of signal verification, adjustment of integration time and data acquisition (Harron & Miller, 1995). Spectral bandpass characterization was performed as in Zarco-Tejada (2000) yielding full-width at half maximum (FWHM) band width estimates of 7.37, 7.15, and 7.25 nm, at 438.5, 546.1 and 576.9 nm, respectively. The fibre spectrometer wavelength calibration was performed using the Ocean Optics HG-1 Mercury-Argon Calibration Source, that produces Hg and Ar emission lines between 253 and 922 nm. Smoothing of reflectance and transmittance was carried out as described in Zarco-Tejada (2000), using a Savitzky-Golay approach with a third-order polynomial function with 40 nm band width.

2.4. Airborne hyperspectral data collection

Compact Airborne Spectrographic Imager (CASI) airborne hyperspectral data were collected over 5 sites of Jack Pine in the Algoma Region, Ontario (Canada), in 1998 and in 1999. The above-canopy data acquisitions were carried out with different spatial and spectral configurations. A *Mapping Mission* with 0.5 m spatial resolution and seven spectral bands was collected for accurate location of the 20 × 20 m study sites. Reflectance imagery used for model inversion in this study were collected in a *Hyperspectral Mission*, with 2 m spatial resolution, 72 channels and 7.5 nm spectral resolution (Fig. 2). Hyperspectral data were processed to *at-sensor* radiance using calibration coefficients derived in the laboratory by the Centre for Research in Earth and Space Technology (CRESTech). Aerosol optical depth at 550 nm was derived from Micro-Tops II sunphotometer (Solar Light, Philadelphia, PA, USA) readings taken in the study area at the time of data acquisition, and subsequently used to process image data to *ground-reflectance* using the CAM5S atmospheric correction model (O'Neill, Zagolski, Bergeron, Royer, Miller, & Freemantle, 1997. Reflectance data were geo-referenced using GPS data collected onboard the aircraft. Final registration of the hyperspectral data was achieved by co-registration to the *Mapping Mission* imagery using visual identification of ground-referenced 1 m white targets, which served to accurately identify the location of the sites.

Mean reflectance values per plot were calculated from the imagery in each study site of 20 × 20 m, targeting crowns by selecting the 25% of pixels with highest reflectance in the NIR. This method, as in Zarco-Tejada (2000), Zarco-Tejada et al. (2001), enables the calculation of mean reflectance per plot with and without targeting crowns to study the effect of the influence of shadows, canopy openings and the direct understory reflectance in the estimation of biophysical parameters by model inversion.

3. Analysis methods and results

3.1. Needle level pigment estimates using leaf model inversion

PROSPECT leaf model (Jacquemoud & Baret, 1990) was used for this study since (i) it is widely validated with several species, (ii) it is less complex than other leaf models, minimizing the number of variables to invert, with

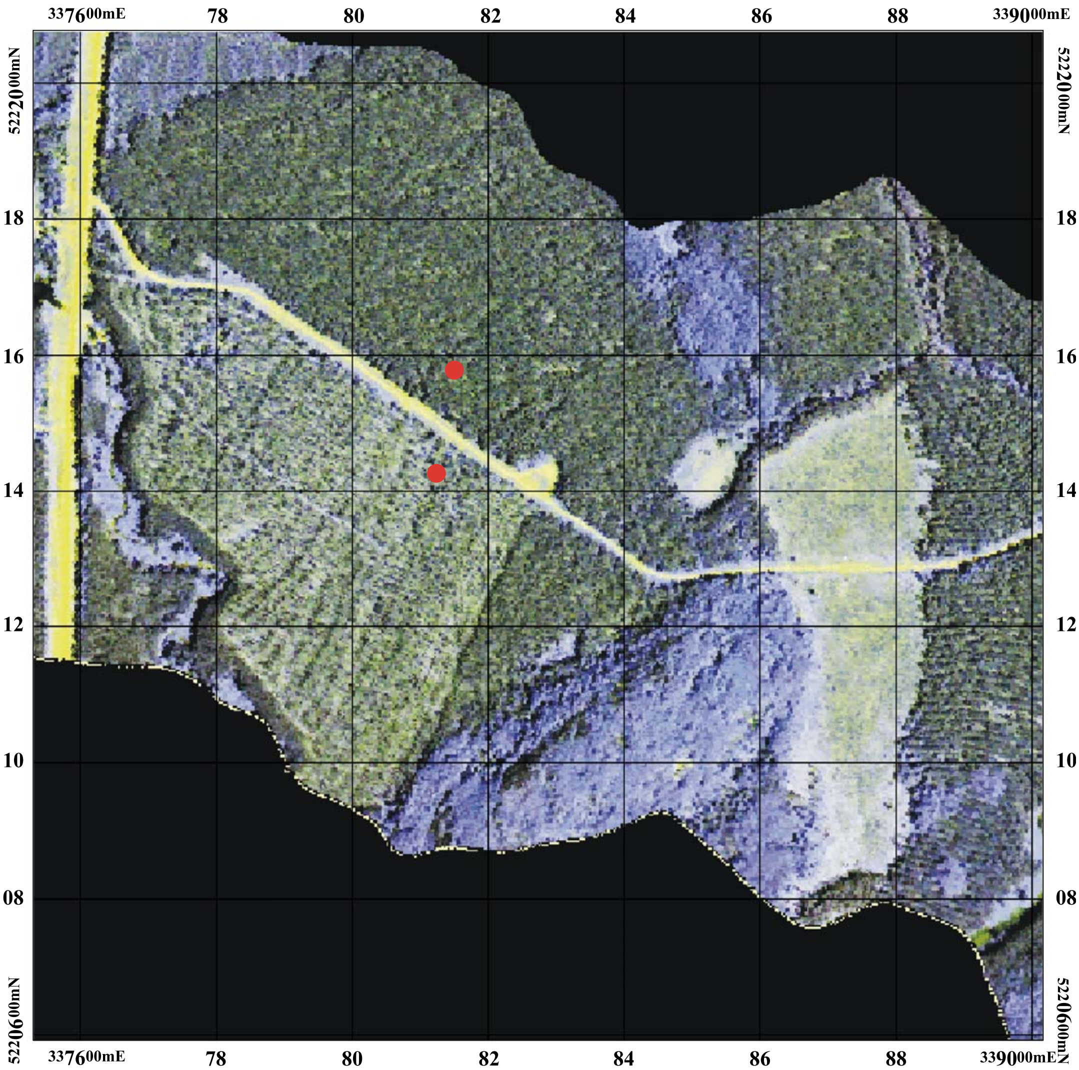

Fig. 2. Airborne hyperspectral CASI image of 72 bands and 2 m spatial resolution collected over two of the 20 × 20 m *Pinus banksiana* Lamb. Study sites used in this study (red circles on the image). Image composite from spectral bands 550 nm (blue), 690 nm (red), and 750 nm (green) from radiometrically calibrated and atmospherically corrected airborne data using 5S model and ground measured aerosol optical depth at 550 nm.

only 4 input parameters and (iii) forward simulations of needle reflectance and transmittance spectra for typical pigment content values showed good agreement in the visible region focus of this study. Fig. 3 (top) shows needle reflectance and transmittance spectra measured with *Harron's method* using a carrier in the Li-Cor integrating sphere and simulated by PROSPECT leaf model. Simulated reflectance and transmittance in the 400–800 nm spectral region requires variation of the two input paramters chl_{a+b} (μg/cm^2) and N (dimensionless), a function of the mesophile structure. The close agreement obtained between measured and simulated reflectance and transmittance spectra in the 400–800 nm spectral region in needles from the study areas is shown in Fig. 3 (top). Measurements of needle reflectance carried out with this methodology also confirm previous work that quantitatively demonstrated the chlorophyll fluorescence effects on leaf apparent reflectance producing a double Gaussian emission using radiative transfer simulation (Zarco-Tejada, Miller, Mohammed, Noland, 2000; Zarco-Tejada, Miller, Mohammed, Noland, & Sampson, 2000a), and in observations under natural illumination conditions (Zarco-Tejada, Miller, Mohammed, Noland, & Sampson, 2000b). The reflectance difference calculated as the measured reflectance minus the modelled reflectance (dashed line) in Fig. 3 (bottom) shows the double emission peak with maxima at 685 and 730 nm due to chlorophyll fluorescence effects on needle apparent reflectance.

A set of 84 Jack Pine shoots from six study sites in July 1999 were used to select 84 groups of 5 single needles to be placed in the carrier for reflectance (r) and transmittance (t) measurement with the Li-Cor integrating sphere. The 84 reflectance and transmittance spectra were used for estimation of the leaf structural parameter N and the total chlorophyll pigment chl_{a+b} using the PROSPECT model. The model inversion was performed by iteration, varying N from

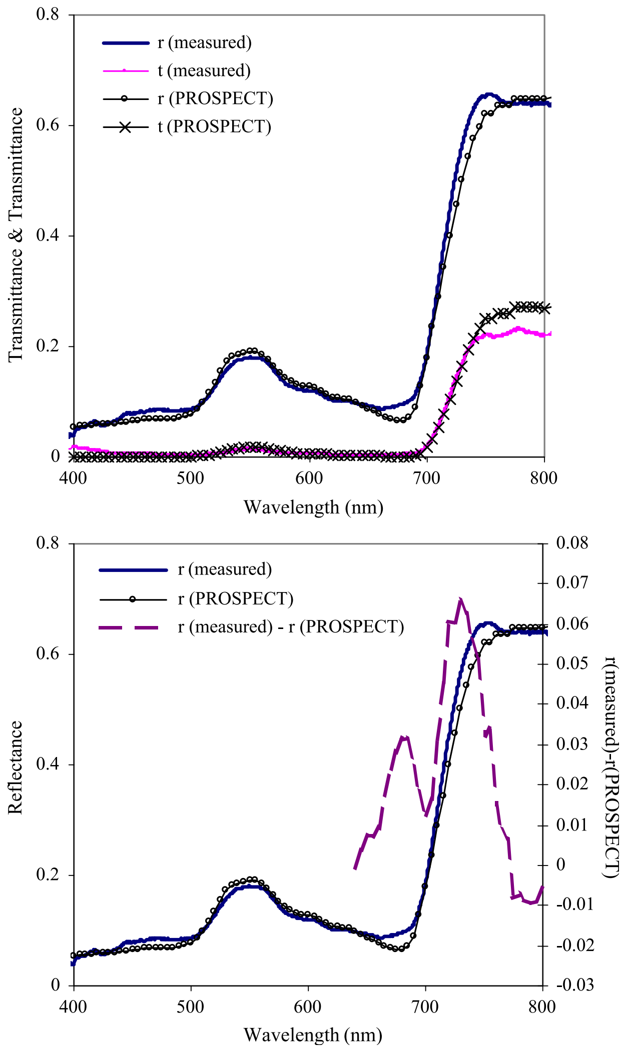

Fig. 3. Needle reflectance and transmittance spectra measured with *Harron's method* using a carrier in the Li-Cor integrating sphere, and simulated by PROSPECT leaf radiative transfer model (top plot). Measured chl_{a+b} in the shoot of the set of needles used for optical measurement of this plot was 60.2 $\mu g/cm^2$ (after conversion using the nominal thickness and SLA). Plotted simulated reflectance and transmittance with PROSPECT was carried out with $\mathrm{chl}_{a+b}=68.5$ $\mu g/cm^2$ and $N=3.5$, obtained previously by numerical inversion of the leaf model. Bottom plot is the reflectance difference calculated as the measured reflectance minus the modelled reflectance (dashed line) showing the double peak with maxima at 685 and 730 nm due to the chlorophyll fluorescence effects on the needle apparent reflectance.

2 to 5 as the first step, with the root mean square error (RMSE) function $\xi(N)$ to be minimized using both r and t in the NIR (780–800 nm), where structural effects dominate significantly over pigment effects in reflectance and transmittance (Eq. 1).

$$\mathrm{RMSE} = \xi(N, \mathrm{chl}_{a+b}) = \sqrt{\frac{\sum_{\lambda}[(r_{\mathrm{PROSPECT}} - r_m)^2_{\lambda} + (t_{\mathrm{PROSPECT}} - t_m)^2_{\lambda}]}{n}} \quad (1)$$

where r_{m} and t_{m} are r and t measured from the needle samples with the Li-Cor sphere and fibre spectrometer. In the second step, with N estimated, chl_{a+b} was varied from 40 to 100 $\mu g/cm^2$ and the function $\xi(N, \mathrm{chl}_{a+b})$ minimized by calculating the RMSE over the 450–700 nm range. Estimated chl_{a+b} in $\mu g/cm^2$ from the inversion of PROSPECT had to be converted into the units of the laboratory-measured chl_{a+b} in μg/g (μg of chl_{a+b} per g of tissue). The conversion was achieved by dividing each PROSPECT estimation ($\mu g/cm^2$) by the product of the measured average needle thickness T_{a} for the five needles in the sample (cm) and the tissue density δ (g/cm^3).

$$chl_{a+b}[\mu g/g] = \frac{chl_{a+b}[\mu g/cm^2]}{T_a[cm] \cdot \delta[g/cm^3]} \quad (2)$$

The live tissue density δ was considered constant for the study and can be considered approximately as:

$$\delta[\mathrm{g/cm^3}] = \frac{1}{\mathrm{SLA}_f[\mathrm{cm}^2/g] \cdot T_n[\mathrm{cm}]} \quad (3)$$

where $\mathrm{SLA_f}$ is the Specific Leaf Area for fresh needles, and T_{n} is the nominal Jack Pine needle thickness. With T_{n} set equal to 0.062 cm based on measurements, and $\mathrm{SLA_f}$ set to 35 cm^2/g, a suitable conversion normalization factor δ in Eq. (2) was achieved for the Jack Pine needles under study. Table 1 shows that this empirically derived $\mathrm{SLA_f}$ value (35 cm^2/g) is reasonable as it is in the range between actual measurements of fresh weight needle specific area and the more usual dry weight specific needle area measure of SLA. Following the above procedure, the assessment of chl_{a+b} estimation by PROSPECT model inversion yielded $r^2=0.4$ (Fig. 4). Chl_{a+b} estimation by model inversion was carried out with thickness T_{n} set to 0.062 cm, and $\mathrm{SLA_f}=35$ cm^2/g. Variation in T_{n} and SLA, which together determine the normalization constant δ, affect the slope, therefore the under/overestimation of chl_{a+b}, but not the determination coefficient obtained by PROSPECT model inversion. The lower determination coefficient obtained at the needle level is thought to be due primarily to errors incurred arising from several factors associated with the difficult optical and biochemical characterization of needles. Among such factors are: (1) the low signal-to-noise ratio obtained in the reflectance and transmittance measurements with the Li-Cor integrating sphere due to the low transmittance through the carrier slots, and particularly, (2) the pigment extraction protocol required tissue from about 20 needles, which did not include the five used for optical measurements which is expected to introduce discrepancies between measured and estimated pigment characterizations. (Steps have been undertaken to rectify these potential difficulties in new experiments with conifers). Nevertheless, Fig. 4 shows that model inversion by radiative transfer can be performed in needles using only two variables, therefore reducing the number of

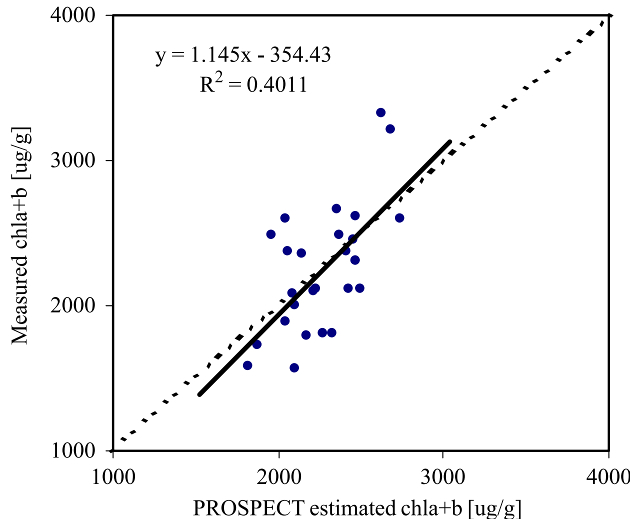

Fig. 4. Estimation of chl_{a+b} (μg/g) in needles collected from Jack Pine study sites by PROSPECT model inversion from needle reflectance and transmittance measurements using the *Harron's method*, with nominal thickness $T_n = 0.062$ cm, and $SLA_f = 35$ cm^2/g.

total parameters to minimize in a leaf model when linked to a complex forest canopy model.

3.2. Canopy modelling for conifer stands

Jack Pine canopy reflectance simulation required a 3-D radiative transfer model to account for complex structural variables needed for an accurate estimation of biophysical parameters. This role was fulfilled by Spreading of Photons for Radiation INTerception (SPRINT) developed by Goel and Thompson (2000). SPRINT employs a ray-tracing/Monte Carlo method, with an added novel photon-spreading concept to provide efficient generation of photon statistics in complex 3-D scenes. SPRINT can be used to calculate bidirectional reflectance and related quantities, such as gap probability, geometric fraction and albedo, for a forest scene created. In this study, SPRINT was used to simulate the reflectance of Jack Pine canopies at the average viewing geometry of the CASI images from the 1998 and 1999 field campaigns. Since the solar zenith angle varied between 29.6° and 38.9° for the 1998 campaign, and between 44.4° and 52.9° for the 1999 campaign, values of 35° and 48° were adopted for the simulations for 1998 and 1999 campaigns, respectively, with view zenith angle 0°.

Scene canopy reflectance was modelled through SPRINT by calculating the optical properties of the elements and major canopy structural parameters. The optical properties of elements include reflectance and transmittance of needles (from the linked PROSPECT model, using *N* estimated by model inversion from the set of needles sampled from the pine sites), reflectance of understory and reflectance of tree trunks. In addition, 10 canopy structural parameters listed in Table 1 were used along with the nominal values for the Jack Pine stands under study.

Soil reflectance was measured at seven spectral bands using the CASI spatial mode of 1 m resolution, and an interpolation was performed to get the soil reflectance for the 72-channel spectral range of CASI instrument in the hyperspectral mode. The reflectance of tree trunk for Jack Pine was taken from Middleton, Walter, et al. (1997) that incidentally is nearly the same as the measured soil reflectance. Shoots are usually considered as the basic scatterers in conifers. The biophysical parameters of shoots of Jack Pine were therefore used instead of the parameters of needles in the simulation. The value of leaf area density was calculated from tree density, crown size and canopy effective LAI as in Chen and Cihlar (1995). Accordingly, canopy reflectance simulation with SPRINT

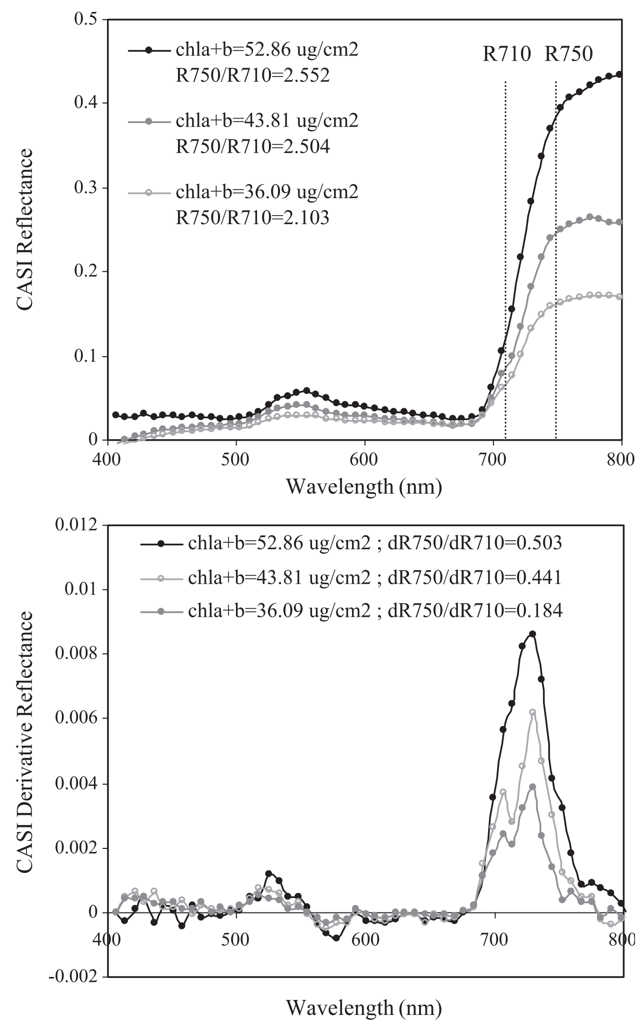

Fig. 5. CASI hyperspectral airborne reflectance spectra from three Jack Pine sites of 20 × 20 m, 2 m spatial resolution and 72 spectral bands. CASI data were radiometrically calibrated and atmospherically corrected using 5S model and ground aerosol optical depth. Canopy reflectance spectra (top plot) and derivative reflectance (bottom plot) are shown from study sites with different ground-measured chl_{a+b}, showing consistent relationship between CASI R750/R710 and ground-measured chl_{a+b}. The double-peak in the derivative reflectance (bottom plot) in the red edge spectral region shows up in stressed vegetation considered due to chlorophyll fluorescence effects.

can be carried out with the described structural parameters, and with needle reflectance and transmittance modelled from PROSPECT.

3.3. Pigment estimates through inversion of linked PROSPECT and SPRINT models

PROSPECT and SPRINT radiative transfer models were linked in order to perform needle chl_{a+b} estimation by numerical model inversion. The 10 mean reflectance spectra calculated from the 2 m CASI reflectance data acquired from the five 20 × 20 m Jack Pine study sites in 1998 and 1999 were used as input for inversion of data from the linked models. Two sets of mean canopy reflectance were used for the model inversion as in Zarco-Tejada (2000) and Zarco-Tejada et al. (2001), one of them targeting crowns, therefore minimizing the effects of shadows and canopy openings, and the other set using all pixels in the 20 × 20 m area, therefore being more affected by structural differences between sites as well as by shadows and canopy openings. The inversion procedure adopted used a minimizing merit function based on the R750/R710 (Zarco-Tejada et al., 2001) optical index, which was highly correlated at both leaf and canopy levels with chlorophyll content. Fig. 5 shows CASI hyperspectral airborne reflectance data (top plot) and derivative reflectance (bottom plot) from three Jack Pine sites with different ground-measured chl_{a+b}. Consistency is found between ground truth pigment at the study sites and canopy reflectance measured with the CASI sensor when using the optical index R750/R710. It can be seen that the direct relationship between R750/R710 and chl_{a+b} content is consistent regardless of the structural differences between sites (Fig. 5, top). The double-peak in the derivative reflectance (Fig. 5, bottom) in the red edge spectral region shows up in stressed vegetation with low chl_{a+b} and is consistent with chlorophyll fluorescence effects on the reflectance.

Table 1 shows the nominal parameters used in the estimation for both PROSPECT and SPRINT models, allowing chl_{a+b} to vary to minimize, by iteration, the merit function based on R750/R710 red edge optical index. Needle chl_{a+b} content estimation by this method from the 10 sites in the 2 consecutive years yielded $r^2 = 0.4$ and RMSE = 8.1 μg/cm^2 when targeting sunlit crown pixels (Fig. 6), and an $r^2 = 0.18$ and RMSE = 10.25 μg/cm^2 when using stand pixels that included shadows and openings. The relationship between chl_{a+b} estimation made by linking PROSPECT and SPRINT models and ground truth obtained a slope close to 1 (0.987) and a small intercept (2.9), indicating that no systematic under/overestimation of pigment content resulted when using such linked models and the nominal structural parameters described for all study sites.

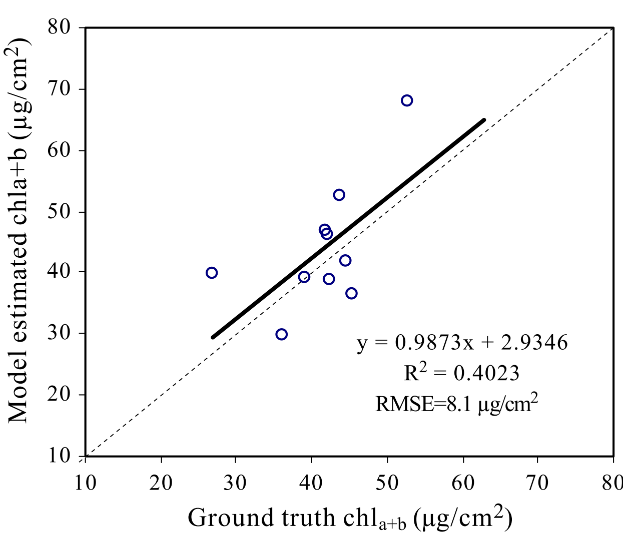

Fig. 6. Relationship between measured and estimated needle chl_{a+b} content by numerical inversion of PROSPECT and SPRINT models, yielding $r^2 = 0.4$ and RMSE = 8.1 μg/cm^2 when targeting sunlit crown pixels. Pigment content was measured from 10 sites in 2 consecutive years with a range of 26.8–56.8 μg/cm^2 (1570–3320 μg/g).

4. Conclusions

Results obtained in this paper indicate the feasibility of estimating needle chl_{a+b} by radiative transfer model inversion of hyperspectral airborne reflectance data acquired from conifer canopies. PROSPECT and SPRINT leaf and canopy models were linked for numerical inversion of canopy reflectance spectra using nominal structural parameters and allowing chl_{a+b} to vary in the minimization process, based on a red edge spectral transform R750/R710 (Zarco-Tejada et al., 2001) as the merit function. Moreover, it is demonstrated that the successful methodology developed with deciduous canopies by linking leaf and canopy radiative transfer models targeting crowns to minimize the effects of shadows and canopy structure can be applied in conifer canopies. Linked PROSPECT and SPRINT models using nominal parameters from the areas of study obtained $r^2 = 0.4$ and RMSE= 8.1 μg/cm^2 when targeting sunlit crown pixels for a pigment content in the range of 26.8–56.8 μg/cm^2 (1570–3320 μg/g). Reasonable estimation with no under/overestimation of chl_{a+b} was obtained, indicating that such models properly simulate biochemical and structural characteristics of both needles and conifer canopies.

These results confirm previous conclusions in deciduous canopies where a red edge index R750/R710 was used in the merit function (Zarco-Tejada, 2000; Zarco-Tejada et al., 2001). Specific red edge indices used in the merit function have been demonstrated to minimize the effect of variable structural parameters on canopy reflectance and the complicating effect of complex canopy 3D heterogeneity on the inversion of radiative transfer models with several input variables.

Harron's method for needle reflectance and transmittance measurement in the 400–800 nm spectral region using a special carrier in the Li-Cor integrating sphere obtained good results when PROSPECT model inversion is performed. This method does not require the careful measurement of the gap fraction between the needles in the port and avoids systematic error due to the effect of the specular scattered light from the curved needle surface when a carrier is used. Needle reflectance and transmittance measured with *Harron's method* from five study sites of Jack Pine were used for chl_{a+b} estimation by PROSPECT model inversion, obtaining $r^2 = 0.4$. The PROSPECT model was used because it is widely validated with several species, it is less complex than other leaf models, minimizing the number of variables to invert, with only four input parameters, and especially since forward simulations of needle reflectance and transmittance spectra for typical pigment content values showed good agreement in the visible region focus of this study. The relatively low determination coefficient at the needle level was potentially affected by errors in the protocol used for biochemical measurements of the needles sampled from the different stands used for this study. Within-shoot pigment variability would have affected the ground-truth mean values of chl_{a+b} from laboratory measurements, as well as the results from extractions carried out on shoots for which the optically measured needles represent only about 10% of the shoot. The impracticality of measuring needle reflectance, transmittance, and pigments from the same needles led to potentially significant discrepancies with the biochemical characterization of the shoots, affecting the determination coefficients obtained at leaf and canopy level by model inversion.

The methodology proposed in this paper of linking needle and canopy radiative transfer models for parameter estimation by inversion can be considered very promising, although further research is needed on the adequacy of the radiative transfer assumptions made at leaf and canopy levels for more accurate simulation of the conifer canopy reflectance.

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