CHLOROPHYLL *a+b* CONTENT ESTIMATION THROUGH TURBID-MEDIUM AND MONTE-CARLO RT MODEL INVERSION FOR FOREST CANOPIES, USING HYPERSPECTRAL DATA

Pablo J. Zarco-Tejada,[1,6] John R. Miller,[1,2] John Harron,[1,7] Baoxin Hu,[2,3] Thomas L. Noland,[4] Narendra Goel,[5] Gina H. Mohammed,[4,8] and Paul H. Sampson[4]

1. Introduction

This paper reports on progress made within the Bioindicators of Forest Sustainability Project (Mohammed *et al.*, 1997; Sampson *et al.*, 1998) to develop links between physiologically-based bio-indicators (e.g., pigment concentrations, chlorophyll fluorescence) from field and laboratory data and optical indices from hyperspectral remote sensing data for assessing forest condition.

Predictions of chlorophyll content (chl_{a+b}) or any other canopy biophysical parameter from airborne or satellite canopy reflectance are generally carried out through four different methodologies: i) directly studying the statistical relationships between ground-measured biochemical data and canopy-measured reflectance (Johnson *et al.*, 1994; Matson *et al.*, 1994); ii) applying the leaf-level relationships derived between optical indices and the pigment content directly to canopy-measured reflectance (Peterson *et al.*, 1988; Yoder and Pettigrew-Crosby, 1995; Zagolski *et al.*, 1996); iii) *scaling-up* the leaf-level relationships based on optical indices related to pigment content through models of canopy reflectance or infinite reflectance (Zarco-Tejada *et al.*, 1999a; 1999b; 2000); and iv) inverting the observed canopy reflectance through a canopy reflectance or infinite reflectance model coupled with a leaf model to estimate the optimum pigment content (Jacquemoud *et al.*, 1995; Kuusk, 1998; Demarez and Gastellu-Etchegorry, 2000; Weiss *et al.*, 2000; Jacquemoud *et al.*, 2000).

Traditional statistical methods have demonstrated successful retrievals of pigment content from hyperspectral reflectance, such as from multivariate analysis between Airborne Visible InfraRed Imaging Spectrometer (AVIRIS) reflectance and total nitrogen, lignin, starch, chlorophyll content and LAI (Johnson *et al.*, 1994) and with nitrogen and chlorophyll (Matson *et al.*, 1994) through application of a stepwise multiple-regression procedure using the AVIRIS spectral bands. Nevertheless, statistical leaf-level relationships applied to canopy reflectance for pigment estimation are site and species specific (Chappelle *et al.*, 1992; Gitelson and Merzylak, 1997) and therefore require relationship parameterization that is a function of the canopy structure and viewing geometry at the time of remote sensing data collection. Therefore, the statistical relationships derived at leaf level need to be parameterized in order to be useful for estimation at the canopy level, due to the differences between the two media: one where the relationship is derived (leaf) and the other where it is applied for estimations (forest canopy). Although significant correlations are found when statistical approaches are used, no prediction capabilities can be inferred from either one of these research results since the locally-derived relationships are affected by species, canopy structure, LAI, canopy openings, shadows and understory.

Scaling-up methods using coupled leaf-level statistical relationships and radiative transfer (RT) models (Zarco-Tejada, *et al.*, 1999a, 1999b; Zarco-Tejada, 2000), and RT model inversion techniques coupling leaf and canopy models (Jacquemoud *et al.*, 1995; Kuusk, 1998; Demarez and Gastellu-Etchegorry, 2000; Jacquemoud *et al.*,

---

[1] Centre for Research in Earth and Space Science, York University, 4700 Keele Street, Toronto M3J 1P3, Canada.
[2] Department of Physics and Astronomy, York University, Toronto M3J 1P3, Canada.
[3] Canadian Space Agency, 6767 Route de L'Aéroport Saint-Hubert, Québec J3Y 8Y9, Canada.
[4] Ontario Forest Research Institute, OMNR, Sault Ste. Marie P6A 2E5, Ontario, Canada.
[5] Department of Computer Science,Wayne State University Detroit, Michigan 48202 USA.
[6] Now at Center for Spatial Technologies and Remote Sensing (CSTARS), Department of Land, Air, and Water Resources (LAWR), University of California, Davis, CA 95616 – 8671 USA - pzarco@ucdavis.edu
[7] Now at Spectral Applied Research Inc., 10 North Rivermede Rd. Concord, Ontario L4K 2H2, Canada.
[8] Now at P&M Technologies, 66 Millwood St., Sault Ste. Marie, Ontario P6A 6S7, Canada.

2000; Zarco-Tejada *et al.*, 2001a; 2001b) allow consideration of the canopy structure, with leaf RT simulation using leaf biochemical constituents as input to model leaf reflectance and transmittance that is in turn used as input for the canopy reflectance model. This paper reports on progress made to estimate leaf chlorophyll content by radiative transfer model inversion techniques. The study was carried out at forest sites of *Pinus strobus* L. and *Acer saccharum* M. in Ontario, Canada, where field measurements and hyperspectral CASI imagery were collected between 1997 and 2000 in airborne deployments. PROSPECT, SAILH, and SPRINT radiative transfer models were used for numerical inversion using red edge spectral indices to build the merit function used in the optimization procedure. Individual tree samples were collected at each site for biochemical analysis and measurement of leaf chlorophyll, carotenoid concentrations, as well as reflectance and transmittance of broad leaves and needles. The model inversion techniques were tested using CASI data of 72 and 288 channels and 0.5 and 2 m spatial resolution.

2. Hyperspectral Data Collection

Data collection was carried out in 18 study sites of *Pinus strobus* L. and *Acer saccharum* M. in Ontario (Canada), where field data and airborne hyperspectral data were collected with the *Compact Airborne Spectrographic Imager* (CASI) sensor. Airborne data were collected in the 400-950 nm spectral range, with spatial resolution varying from 0.5 to 5m and with CASI modes of operation of 72 and 288 bands with 7.5 and 2.5 nm spectral resolution, respectively. Field campaigns were carried out in summer of 1997, 1998, 1999 and 2000, collecting LAI, canopy cover, using hemispherical photography and PCA-LiCor 2000. A total of 440 leaf samples per year were collected from 12 deciduous sites and 84 groups of needles from the 6 conifer sites. Leaf and needle samples were used for measuring chlorophyll *a+b* and carotenoids as described in Zarco-Tejada *et al.* (2000). Reflectance (*r*) and transmittance (*t*) from each broad leaf and needle sample were obtained with a LiCor integrating sphere attached to a 7.5 nm bandwidth fibre spectrometer in the 400-900 nm range. Raw CASI data were calibrated to radiance and atmospherically corrected using CAM5S model using aerosol optical depth at 550nm collected over the area at the time of airborne data collection. Airborne data were geocoded using onboard GPS and two-axis gyro.

3. Leaf-Level Radiative Transfer Modelling for Broad Leaves and Needles

Accurate determination of the optical properties of leaf samples is critical for development and validation of leaf RT models. The PROSPECT model (Jacquemoud and Baret, 1990), has been widely used and validated in broadleaves for numerical inversion to estimate chlorophyll content. Nevertheless, development and validation of leaf models to simulate needle reflectance and transmittance has not been that successful due to existing difficulties to measure the optical properties of needles associated with their shape and size.

The method of Daughtry *et al.* (1989) for needle *r* and *t* was adapted by Harron and Miller (Harron, 2000) through the use of a carrier to support the needles avoiding gaps between samples. Using the carrier-based method the effect of the specular-scattered light is eliminated completely, therefore avoiding errors made in the meticulous measurement of the gap fraction between the needles presented at the exit port. Besides, Harron and Miller's method avoids the influence of specular scattered light from the curved needle surface which in previous methods escapes from the sphere in the reflectance measurements and is introduced into the sphere in the transmittance measurements. This new method considerably improved the measurement of needle optical properties (Harron, 2000) and allowed successful application of PROSPECT model to simulate needle *r* and *t*. Figure 1 shows needle reflectance and transmittance spectra measured with Harron and Miller's method using a carrier in the Li-Cor integrating sphere, and simulated by PROSPECT leaf model using chl_{a+b} and N values obtained by model inversion. The close agreement obtained between measured and simulated reflectance and transmittance spectra in needles from the study areas, and the extensive validation of PROSPECT in the literature prompted our adoption of the traditional PROSPECT for the needle simulations presented in this paper.

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 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 [Equation 1].

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

where r_m and t_m are r and t measured from the needle samples with the Li-Cor and fibre spectrometer. In the second step, with N estimated, chl_{a+b} was varied from 40 to 100 μg/cm^2 and the function $\xi(N, chl_{a+b})$ minimized by calculating the RMSE over the 450-700 nm range. Following the above procedure, the assessment of chl_{a+b} estimation by PROSPECT model inversion yielded r^2=0.4.

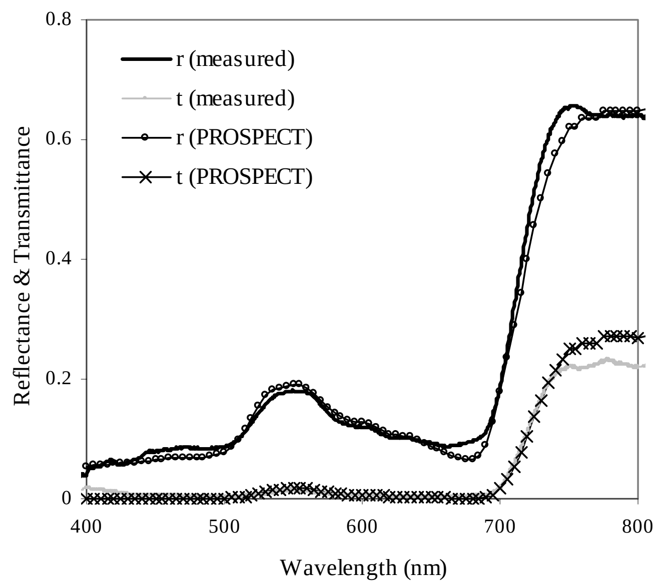

Figure 1. Needle reflectance and transmittance spectra measured with Harron and Miller's method using a carrier in the Li-Cor integrating sphere, and simulated by PROSPECT leaf RT model. Measured chl_{a+b} in the shoot of the set of needles used for optical measurement of this plot was 60.2 μg/cm^2 (after conversion using nominal thickness and FLA). Plotted simulated reflectance and transmittance with PROSPECT was carried out with chl_{a+b} = 68.5 μg/cm^2 and N=3.5, obtained previously by numerical inversion of the leaf model.

4. Estimation of Chlorophyll *a+b* by RT Model Inversion from Airborne Hyperspectral Data in Deciduous and Conifer Canopies

Canopy simulation modeling was carried out using two radiative transfer models, SAILH for closed deciduous canopies, and SPRINT for conifers. The use of turbid-medium models such as SAILH in deciduous canopies was carried out by building a merit function based on spectral transforms to minimize the forest canopy structure, shadows and openings. Building merit functions based on spectral transforms or vegetation indices (Zarco-Tejada, 2000; Zarco-Tejada *et al.*, 2001a) are found effective when they are based on optical indices that are related with the variable subject to estimation, such as chl_{a+b}. The use of optical indices in the merit function has not been reported in any of the validation work found in the literature, although it appears that there is significant inherent potential of this approach in remote sensing application. Reflectance values measured from airborne or satellite sensors are a function of illumination, canopy structure, and atmospheric condition at the time of data collection. On the other hand, estimation of biophysical parameters through optical indices enable the sensitivity to such biophysical parameters to be maximized, normalizing external effects due to atmosphere, illumination conditions, and viewing geometry (Running *et al.*, 1994; Huete and Justice, 1999).

The iterative-optimization numerical model-inversion technique to estimate chlorophyll content by using a coupled leaf model and a canopy model requires the error calculation by comparison of estimated canopy reflectance r^* to the at-sensor measured reflectance r_m. Error calculation consists of determination of a set of parameters $P=(N,Chl_{a+b},C_w,LAI,\theta_s\ldots)$ which minimizes a merit function Δ^2 over the whole spectrum [Equation 2].

$$\Delta^2 = \sum_n [r_m(\lambda_i) - r^*(\lambda_i, P)]^2 \qquad [2]$$

where, $r_m(\lambda_i)$ is the measured canopy spectral reflectance; and $r^*(\lambda_i, P)$ is the modelled canopy spectral reflectance with a set of P parameters. Equation [3] presents the merit function used in this study when the red-edge spectral parameter R_{750}/R_{710} is used for pigment estimation:

$$\Delta^2 = \left[\left(\frac{R750}{R710}\right)_m - \left(\frac{R750}{R710}, P\right)_*\right]^2 \qquad [3]$$

where $R750/R710_m$ is the optical index calculated from measured canopy reflectance, and $R750/R710_*$ is the optical index calculated from modelled canopy reflectance, for a given set of input parameters *P*. Zarco-Tejada *et al.* (2001a) demonstrated that forest canopy shadows and heterogeneity are minimized when a red edge optical index is used in the merit function used for error assessment in the coupled PROSPECT+SAILH RT models. This methodology was used for model inversion in deciduous and coniferous study sites, using PROSPECT+SAILH for deciduous and PROSPECT+SPRINT for coniferous sites. Structural parameters and viewing geometry values for RT modeling (Figure 2) were measured in the field at the time of data collection, with specific pine values extrapolated from field measurements made earlier (Fox, 1991). The structural values from both species were used for model simulation, using the following for *Pinus strobus*: tree density, 1100 trees/ha; Poisson distribution of trees; irregular ellipsoidal crown shape, height of trunk, 8.5 m; height of tree, 15.0 m; trunk radius, 8.3 cm; crown radius, 2.0 m; spherical leaf angle distribution; shoot area, 0.0008 m^2; canopy effective LAI, 2.5; and leaf area density, 0.4171 /m. whereas for *Acer saccharum* parameters were: LAI=3.5, plagiophile leaf angle distribution function (LADF), soil reflectance data derived from CASI imagery, and model-estimated skylight irradiance fraction based on conditions during airborne acquisitions. Estimated versus measured leaf pigment content results from the 12 study sites of *Acer saccharum* yielded r^2=0.4, RMSE=5.5 μg/cm^2 (years 1999 and 2000), and r^2=0.4, RMSE=8.1 μg/cm^2 for *Pinus strobus* (year 2000).

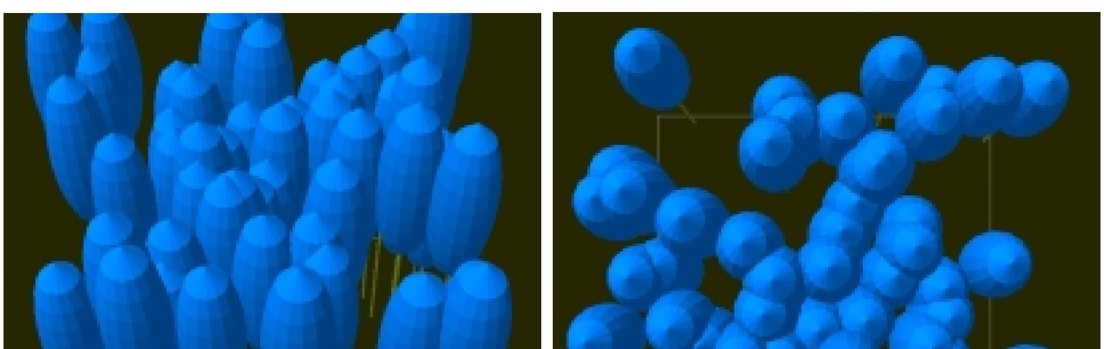

Figure 2. Scene representation of the *Pinus strobus* coniferous canopy used for the Monte-Carlo radiative transfer simulation with SPRINT model (30° viewing angle, left; nadir view, right). Structural parameters and viewing geometry values were measured in the field at the time of data collection for *Pinus strobus*: tree density, 1100 trees/ha with Poisson distribution; irregular ellipsoidal crown shape, height of trunk, 8.5 m; height of tree, 15.0 m; trunk radius, 8.3 cm; crown radius, 2.0 m; spherical leaf angle distribution; shoot area, 0.0008 m^2; canopy effective LAI, 2.5; and leaf area density, 0.4171 /m.

5. Conclusions

This paper demonstrates that radiative transfer model inversion techniques can be applied successfully to forest canopies with different structural characteristics, such as *Acer saccharum* and *Pinus strobus*. The new approach of Harron and Miller for measuring the optical properties of needles using a carrier method, enabled the validation of PROSPECT leaf model for pigment content estimation by inversion in needles. Estimation of chlorophyll content in closed deciduous canopies was successfully carried out using a turbid-medium model (SAILH) coupled to PROSPECT, and building the merit function with a red edge optical index R750/R710. It was previously demonstrated that a turbid-medium model could successfully be used in closed forest canopies when a red edge index is used in the merit function used for minimization. Red edge indices such as R750/R710 used as merit function minimizes shadows and canopy openings, therefore enabling the use of less complicated RT models such as SAILH in forest canopies. The same approach was carried out for the coniferous canopies, coupling PROSPECT to SPRINT Monte-Carlo RT model and using the same red edge index to build the merit function. Results obtained from the 12 study sites of *Acer saccharum* were r^2=0.4, RMSE=5.5 µg/cm^2 (1999 and 2000 campaigns) and r^2=0.4, RMSE=8.1 µg/cm^2 for *Pinus strobus* (2000 campaign), showing that RT model inversion methods can be used with success over forest canopies to estimate chlorophyll content.

6. References

Chappelle, E. W., Kim, M. S. and McMurtrey, J. E. I. (1992), Ratio analysis of reflectance spectra (RARS): an algorithm for the remote estimation of the concentrations of chlorophyll *a*, chlorophyll *b*, and carotenoids in soybean leaves. *Remote Sensing of Environment.* 39:239-247.

Daugherty, C. S. T., Biehl, L. L., and Ranson, K. J. (1989), A new technique to measure the spectral properties of conifer needles, *Remote Sensing of Environment*, 27:81-91.

Demarez, V., and Gastellu-Etchegorry, J.P., (2000) A Modeling Approach for Studying Forest Chlorophyll Content. *Remote Sensing of Environment*, 71:226-238.

Fox, B. (1991), Silvicultural demonstration areas of the Kirkwood Forest. Ministry of Natural Resources, Cent. Ont. For. Tech. Dev. Unit. Blind River, ON, COFTDU Rep. No. 16. 85 pp.

Gitelson, A. A. and Merzlyak, M. N. (1997), Remote estimation of chlorophyll content in higher plant leaves. *International Journal of Remote Sensing.* 18:2691-2697.

Harron, J. W. (2000), Optical properties of phytoelements in conifers, M. Sc. Thesis, *Graduate Program in Earth and Space Science*, pp193, York University, Toronto, December, 2000.

Huete, A., and Justice, C., (1999), MODIS Vegetation Index (MOD 13) Algorithm Theoretical Basis Document, Greenbelt: NASA Goddard Space Flight Centre, http://modarch.gsfc.nasa.gov/MODIS/LAND/#vegetation-indices, 129pp.

Jacquemoud, S. and Baret, F. (1990), Prospect: A model of leaf optical properties spectra, *Remote Sensing of Environment*. 34**:**75-91.

Jacquemoud, S., Baret, F., Andrieu, B., Danson, F. M. and Jaggard, K. (1995), Extraction of vegetation biophysical parameters by inversion of the PROSPECT+SAIL models on sugar beet canopy reflectance data. Application to TM and AVIRIS sensors. *Remote Sensing of Environment.* 52:163-172.

Jacquemoud, S., Bacour, C., Poilve, H., and Frangi, J.P., (2000) Comparison of four radiative transfer models to simulate plant canopies reflectance–Direct and inverse mode, *Remote Sensing of Environment,*74:471-481.

Johnson, L. F., Hlavka, C. A. and Peterson, D. L. (1994), Multivariate analysis of AVIRIS data for canopy biochemical estimation along the Oregon transect. *Remote Sensing of Environment.* 47:216-230.

Kuusk, A. (1998), Monitoring of vegetation parameters on large areas by the inversion of a canopy reflectance model. *International Journal of Remote Sensing.* 19:2893-2905.

Matson, P., Johnson, L., Billow, C., Miller, J. and Pu, R. (1994), Seasonal patterns and remote spectral estimation of canopy chemistry across the Oregon transect. *Ecological Applications.* 4:280-298.

Mohammed, G.H., Sampson, P. H., Colombo, S. J., Noland, T. L., y Miller, J. R. (1997), Bioindicators of forest sustainability: *Development of a forest condition rating system for Ontario*, OFRI, ON, Canada.

Peterson, D. L., Aber, J. D., Matson, P. A., Card, D. H., Swanberg, N., Wessman, C. and Spanner, M. (1988), Remote sensing of forest canopy and leaf biochemical contents. *Remote Sensing of Environment.* 24:85-108.

Running, S.W., Justice C.O., Solomonson, V., Hall, D., Barker, J., Kanfmann, Y.J., Strahler, A.H., Huete, A.R., Muller, J.P., Vanderbilt, V., Wan, Z.M., Teilletland, P. and Carneggie, D., (1994), Terrestrial Remote Sensing and Algorithms Planned for EOS/MODIS, *International Journal of Remote Sensing*, 15(17):3587-3620.

Sampson, P.H., G.H. Mohammed, S.J. Colombo, T.L. Noland, J.R. Miller and P.J. Zarco-Tejada, 1998. *Bioindicators of Forest Sustainability Progress Report, Ontario Forest Research Institute*, Sault Ste. Marie, ON, Canada.

Weiss, M., Baret, F., Myneni, R.B., Pragnere, A. and Knyazikhin, Y., (2000) Investigation of a model inversion technique to estimate canopy biophysical variables from spectral and directional reflectance data, *Agronomie* 20:3-22.

Yoder, B. J. and Pettigrew-Crosby, R. E. (1995), Predicting nitrogen and chlorophyll content and concentrations from reflectance spectra (400-2500 nm) at leaf and canopy scales. *Remote Sensing of Environment.* 53:199-211.

Zagolski, F., Pinel, V., Romier, J., Alcayde, D., Fotanari, J., Gastellu-Etchegorry, J. P., Giordano, G., Marty, G., and Joffre, R. (1996), Forest canopy chemistry with high spectral resolution remote sensing. *International Journal of Remote Sensing.* 17:1107-1128.

Zarco-Tejada, P. J. (2000), Hyperspectral remote sensing of closed forest canopies: Estimation of chlorophyll fluorescence and pigment content, Ph.D. Dissertation, *Graduate Program in Earth and Space Science*, York University, Toronto.

Zarco-Tejada, P. J., Miller, J. R., Mohammed, G. H., Noland, T. L. and Sampson, P. H. (1999a), Canopy Optical Indices from Infinite Reflectance and Canopy Reflectance Models for Forest Condition Monitoring: Application to Hyperspectral CASI data, In *IEEE 1999 International Geoscience and Remote Sensing Symposium, IGARSS'99*, Hamburg (Germany).

Zarco-Tejada, P. J., Miller, J. R., Mohammed, G. H., Noland, T. L. and Sampson, P. H. (1999b), Optical Indices as Bioindicators of Forest Condition from Hyperspectral CASI data, In Proceedings 19th Symposium of the European Association of Remote Sensing Laboratories (EARSeL), Valladolid (Spain).

Zarco-Tejada, P. J., Miller, J. R., Mohammed, G. H., Noland, T. L and Sampson, P.H. (2000). Chlorophyll Fluorescence Effects on Vegetation Apparent Reflectance: II. Laboratory and Airborne Canopy-Level Measurements with Hyperspectral data, Remote Sensing of Environment, 74(3).

Zarco-Tejada, P.J., J.R. Miller, G.H. Mohammed, T.L. Noland and P.H. Sampson, *Scaling-up* and *Model Inversion* methods with narrow-band Optical Indices for Chlorophyll Content Estimation in closed Forest Canopies with Hyperspectral Data. *IEEE Transactions on Geoscience and Remote Sensing, Special Issue on Hyperspectral Remote Sensing,* in press (2001a).

Zarco-Tejada, P.J., J.R. Miller, Harron, J., Hu, B., Noland, T.L., Goel, N., Mohammed, G.H., and P.H. Sampson, Needle Chlorohyll content estimation through model inversion using hyperspectral data from Boreal Conifer Forest Canopies. *Remote Sensing of Environment,* BOREAS Special Issue III (submitted, 2001b).