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## PROSPECT + SAIL models: A review of use for vegetation characterization

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#### ABSTRACT

The combined PROSPECT leaf optical properties model and SAIL canopy bidirectional reflectance model, also referred to as PROSAIL, has been used for about sixteen years to study plant canopy spectral and directional reflectance in the solar domain. PROSAIL has also been used to develop new methods for retrieval of vegetation biophysical properties. It links the spectral variation of canopy reflectance, which is mainly related to leaf biochemical contents, with its directional variation, which is primarily related to canopy architecture and soil/vegetation contrast. This link is key to simultaneous estimation of canopy biophysical/structural variables for applications in agriculture, plant physiology, or ecology, at different scales. PROSAIL has become one of the most popular radiative transfer tools due to its ease of use, general robustness, and consistent validation by lab/field/space experiments over the years. However, PROSPECT and SAIL are still evolving: they have undergone recent improvements both at the leaf and the plant levels. This paper provides an extensive review of the PROSAIL developments in the context of canopy biophysics and radiative transfer modeling.

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## 1. Introduction

From the beginning of optical remote sensing, radiative transfer models have helped in the understanding of light interception by plant canopies and the interpretation of vegetation reflectance in terms of biophysical characteristics. Since they attempt to describe absorption and scattering, the two main physical processes involved in such a medium, canopy radiative transfer models are useful in designing vegetation indexes, performing sensitivity analyses, and developing inversion procedures to accurately retrieve vegetation properties from remotely sensed data. Among all the codes published during the last two decades (see for instance Liang, 2003), the SAIL canopy bidirectional reflectance model and the PROSPECT leaf optical properties model are the most popular. An analysis based on the ISI (Institute of Science Information) Web of Science finds a total of 113 and 105 articles using PROSPECT and SAIL, respectively, that have been pub-

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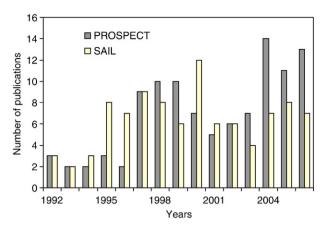
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lished since 1992, showing parallel evolution of the models (Fig. 1). They score 1675 and 1783 citations both with an h-index (number of papers h with at least h citations each) between 23 and 24. PROSPECT combined with SAIL are used in 29 articles with 513 citations leading to 18 citations per article, slightly higher than PROSPECT (15) and SAIL (16) separately. This confirms the importance of these two models in the scientific community and their close relations.

Linking these models into PROSAIL about sixteen years ago allowed description of both the spectral and directional variation of canopy reflectance as a function of leaf biochemistry — mainly chlorophyll, water, and dry matter contents — and canopy architecture — primarily leaf area index, leaf angle distribution, and relative leaf size. The principles on which PROSAIL is founded have been extensively tested, which partly explains its success.

In this review, we will focus on the foundations of PROSPECT and SAIL and their applications, with special emphasis on the coupled PROSAIL model. The first section is an overview of the model principles and time evolution. Then we will see how one can use these models to generate databases and test new spectral indexes, or to perform sensitivity analyses intended to highlight the main canopy biophysical variables that contribute to spectral and directional reflectance variability. In the third section, we report research

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**Fig. 1.** Number of publications per year retrieved from the ISI Web of Science for PROSPECT (query = 'PROSPECT' & 'leaf') and SAIL (query = 'SAIL' & 'reflectance') during the period 1992–2007.

activities evaluating PROSAIL. Finally, applications of the models are listed, with a special focus on techniques used to retrieve canopy biophysical variables from remote sensing observations (iterative methods, look-up tables, artificial neural networks, etc.). We draw conclusions on the future of PROSAIL, both in terms of the required evolution of radiative transfer models and their application.

#### 2. Model overview

Now in widespread use in the remote sensing community, SAIL (Scattering by Arbitrary Inclined Leaves) is one of the earliest canopy reflectance models (Verhoef, 1984, 1985). It is an extension of the 1-D model developed by Suits (1972) to simulate the bidirectional reflectance factor (see Schaepman-Strub et al., 2006, for details on radiometric definitions of reflectance) of turbid medium plant canopies, by solving the scattering and absorption of four upward/ downward radiative fluxes. SAIL actually provides all four-stream optical properties (nine in total) of the canopy layer at the output (Verhoef, 1985). It has given rise to several derivative versions: to describe vertically heterogeneous canopies, multi-layer (vertical gradients of leaf optical properties) and multi-element one-dimensional models have been proposed such as GeoSAIL (Verhoef & Bach, 2003b) or 2M-SAIL (Weiss et al., 2001); the hot-spot effect was added in SAILH after a formalism by Kuusk (1991) as a function of the ratio of leaf size to canopy height; a numerically robust and speed-optimized version of the model called 4SAIL was recently published by Verhoef et al. (2007); in order to simulate horizontally discontinuous canopies, the SAIL model was also combined with geometric models like in GeoSail where protrusions are either cylinders or cones allowing inclusion of some clumping at the canopy scale (Huemmrich, 2001); and more recently, Verhoef and Bach (2007) proposed an extension of GeoSAIL (not to be confused with GeoSail) including crown clumping, called 4SAIL2, that was additionally combined with PROSPECT and a soil BRDF model based on Hapke's work (Hapke, 1981; Hapke & Wells, 1981). Besides this gradual improvement and parallel increase in complexity, the SAIL formalism was adapted to include emission in the radiative transfer processes: solar-induced chlorophyll a fluorescence emission was added in FLSAIL (Rosema et al., 1991) and FluorSAIL (Miller et al., 2005), and thermal emission in 4SAIL (Verhoef et al., 2007) to simulate canopy brightness temperature in a consistent way with that used for reflectance.

At the leaf level, PROSPECT pioneered the simulation of directional-hemispherical reflectance and transmittance (Schaepman-Strub et al., 2006) of various green monocotyledon and dicotyledon species, as well as senescent leaves, over the solar spectrum from 400 nm to 2500 nm (Jacquemoud & Baret, 1990). It is based on the

Allen et al. (1969) representation of the leaf as one or several absorbing plates with rough surfaces giving rise to isotropic scattering. The model uses two classes of input variables: the leaf structure parameter N which is the number of compact layers specifying the average number of air/cell walls interfaces within the mesophyll, and the leaf biochemical content, which has changed since the original formulation of the model (Fourty et al., 1996; Jacquemoud et al., 1996, 2000). The absorption of light by photosynthetic pigments which predominates in the visible (VIS) spectrum was long assumed to be entirely caused by chlorophylls, although carotenoids (including xanthophyll pigments) and anthocyanins may be significant in greening or senescing leaves. Feret et al. (2008) recently succeeded in separating total chlorophylls from total carotenoids which, potentially, will significantly enhance the ability of remote sensing data to estimate photosynthetic rates and more accurate monitoring of vegetation stress. To paint a complete picture of the situation, Bousquet et al. (2005) included a physical description of directional reflectance properties of leaves, adding the contribution of specular reflection on leaf surface to the original Lambertian fluxes; differences in adaxial and abaxial optical properties were introduced in the model by including absorption and scattering gradients in the leaf blade (Kai et al., in press); finally, a new version calculating steady-state chlorophyll a fluorescence is underway (Pedrós et al., submitted for publication).

#### 3. Coupling of PROSPECT and SAIL: PROSAIL

The first model inversions of SAIL, performed by Goel (1989), allowed estimates of canopy architecture (LAI, leaf angle distribution) on soybean by using field bidirectional reflectance measurements acquired in band 4 (0.8-1.1 µm) of the Exotech Model 100 Radiometer, for 12 solar directions. Currently, few spaceborne instruments have the capability of monitoring the Earth surface with such a directional coverage. Only CHRIS, MISR or PARASOL provide simultaneously along one track data in 5, 9, or up to 16 directions of observation, respectively. Indeed, unless multi-temporal acquisitions are available, most sensors measure the Earth's radiance in several wavebands and one direction, generally at near nadir. However, multispectral or hyperspectral data cannot be inverted by SAIL alone because the increase in the number of wavebands rapidly leads to an under-determined system. Since leaf reflectance, leaf transmittance, and soil reflectance are three wavelength-dependent input variables of SAIL, the implementation of this model to retrieve biophysical variables from canopy reflectance spectra at given solar and viewing angles in a defined relative azimuthal plane requires at least three times as many variables as wavelengths. As a consequence, the inversion of SAIL is generally impracticable unless several viewing angles are available. To reduce the dimensionality of the inverse problem and to assess the canopy biochemistry, SAILH was coupled with PROSPECT early in the 1990's to derive PROSAIL (Baret et al., 1992). This was the beginning of a long series of published literature. The main input variables of the integrated model are shown in Table 1 and Fig. 2 sketches the actual coupling. Note that the output variables do not confine to the bidirectional reflectance  $\rho_{\rm c}$  but extend to fAPAR and albedo which are key variables in processes describing the exchanges of mass and energy between the canopy and the atmosphere. The coupling simply consists in passing the output leaf reflectance and transmittance of the PROSPECT model into the SAIL model to simulate the whole spectrodirectional canopy reflectance field. The soil spectral or directional reflectance is also required as input of SAIL: field radiometric data are generally used, less often a soil BRDF model. The input variables of Hapke's model (Jacquemoud et al., 1992) are listed in Fig. 2: single scattering albedo  $\alpha(\lambda)$ , phase function  $P(\theta)$ , and surface roughness parameter h. Finally, the topof-atmosphere apparent radiance  $L_0$  in the direction of viewing can S. Jacquemoud et al. / Remote Sensing of Environment xxx (2009) xxx-xxx

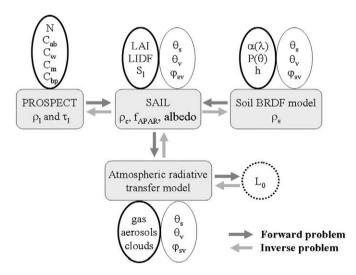
**Table 1**Main variables of PROSAIL.

Model	Symbol	Quantity	Unit
PROSPECT	N	Leaf structure parameter	-
	$C_{ab}$	Chlorophyll $a + b$ content	μg cm <sup>-2</sup>
	$C_{w}$	Equivalent water thickness	cm
	$C_{\rm m}$	Dry matter content	${\rm g~cm^{-2}}$
	$C_{\rm bp}$	Brown pigments content	-
SAIL	LAI	Leaf area index	-
	LIDF*	Leaf inclination distribution function	-
	$s_{\rm L}$	Hot spot parameter	-
	$ ho_{s}$	Soil reflectance assumed Lambertian or not	_
	SKYL	Ratio of diffuse to total incident radiation	_
	sza or $\theta_{\rm s}$	Solar zenith angle	deg
	vza or $\theta_{\rm v}$	Viewing zenith angle	deg
	raa or $\phi_{sv}$	Relative azimuth angle	deg

<sup>\*</sup>Several functions have been proposed to define the LIDF: polynomial, ellipsoidal or elliptic distribution characterized by an average leaf angle (ALA), Beta distribution characterized by two parameters (a and b).

be computed using an atmospheric radiative transfer model (Baret et al., 1992; Verhoef & Bach, 2007).

PROSPECT has been coupled with most subsequent versions of SAIL that have been adapted to account for some heterogeneity within the vegetation canopy: GeoSail (Bowyer & Danson, 2004; Koetz et al., 2004), GeoSAIL (Verhoef & Bach, 2003a,b), 2M-SAIL (Weiss et al., 2001; Le Maire et al., 2008), 4SAIL (Verhoef, 2005), or 4SAIL2 (Verhoef & Bach, 2007). It has been also integrated into other canopy reflectance models: FCR (Fast Canopy Reflectance, Kuusk, 1994), NADIM (New Advanced Discrete Model, Jacquemoud et al., 2000; Ceccato et al., 2002), MCRM (Markov-Chain Canopy Reflectance Model, Kuusk, 1995) adapted for row crops (Cheng et al., 2006), DART (Discrete Anisotropic Radiative Transfer, Demarez & Gastellu-Etchegorry, 2000), SPRINT (Spreading of Photons for Radiation INTerception. Zarco-Tejada et al., 2004a), FLIM (Forest Light Interaction Model, Zarco-Tejada et al., 2004b), and FLIGHT (three-dimensional Forest LIGHT interaction, Koetz et al., 2004). The last four models are used to simulate discontinuous forest canopies. Similar leaf-canopy coupled models were attempted by Ganapol et al. (1999) with LEAFMOD + CANMOD, Dawson et al. (1999) with LIBERTY + FLIGHT, and Dash and Curran (2004) with LIBERTY + SAIL. However, the distribution of these codes in the remote sensing community has remained limited compared to PROSAIL.

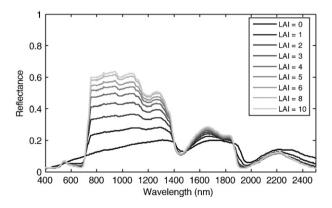


**Fig. 2.** The PROSAIL model: coupling of SAIL and PROSPECT radiative transfer models to simulate canopy spectral and directional reflectance in the forward and inverse directions. Input variables are listed in white ellipses, models and output variables are embedded in gray boxes.

### 4. Sensitivity analysis with PROSAIL

Model simulations help quantify the contribution of canopy biophysical and biochemical properties to canopy reflectance. One of the first applications of PROSAIL focused on the red edge (Baret et al., 1992; Broge & Leblanc, 2000). From the beginning of imaging spectrometry, this portion of the reflectance spectrum between the red and the near-infrared, which switches from concave to convex and then gives rise to an inflexion point, has been a focus of research and development in hyperspectral remote sensing. PROSAIL numerical simulations showed that the spectral shifts in this wavelength window were mainly produced by variations in leaf chlorophyll and leaf area index. Moreover, the wavelength position of the inflexion point was found to be almost insensitive to soil substrate and atmospheric conditions, giving this index an advantage over many previous vegetation indexes. Interestingly, Le Maire et al. (2004) who used a 1 nm resolution version of PROSPECT revealed the existence of a sudden jump of the red edge position from ~695 nm to ~725 nm when chlorophyll exceeded  $45 \, \mu g \, cm^{-2}$ . This was attributed to nearby chlorophyll a absorption peaks (at 679 and 703 nm). Although the inflexion point per se seems to be no longer a useful indicator, the red edge properties still remain characteristic of plant chlorophyll content (Le Maire et al., 2008).

By successively changing PROSAIL input variables, Jacquemoud (1993) performed a simple sensitivity analysis which revealed that N only slightly changed canopy reflectance over the whole solar domain, and that LAI and the average leaf angle (ALA) of the LIDF produced similar effects in the model. As a result, identification of these three variables appeared to be problematic. Fig. 3 presents a simple but instructive simulation of PROSAIL intended to show how sensitive the reflectance of a plant canopy is to variation in LAI from 0 (bare soil) to 10 (very dense vegetation). All other variables are kept constant to highlight canopy reflectance changes due to LAI variation only. Such a situation is highly unlikely under natural conditions because canopy biophysical variables in a given ecosystem often co-vary. For instance, when foliage is packed more densely in a canopy, the biochemical composition of leaves changes, although more or less predictably. Nonetheless, Fig. 3 demonstrates the well accepted notion that an increase of LAI induces a decrease of reflectance in the red and an increase in the near infrared (NIR), but this occurs with no noticeable effects in the shortwave infrared (SWIR) at 1450 nm where water absorption is maximal. The small influence in the green is attributable here to the darkness of the soil but it may increase when using a brighter soil background. Fig. 3 illustrates how vegetation indexes based on the red and NIR wavebands of optical sensors make use of these remarkable properties to quantify LAI. Other indexes have been designed to correlate with canopy water content by combining reflectances in the NIR and SWIR at ~1200 nm. Contrary to the VIS,

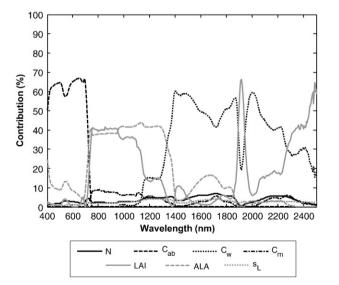


**Fig. 3.** Effect of LAI on canopy reflectance using PROSAIL ( $\theta_s$  = 20°,  $\theta_v$  = 0°,  $\varphi_{sv}$  = 0°, horizontal visibility = 100 km, LIDF = spherical,  $s_L$  = 0.25, N = 1.5,  $C_{ab}$  = 50  $\mu g$  cm $^{-2}$ ,  $C_w$  = 0.01 cm, and  $C_m$  = 0.005 g cm $^{-2}$ ).

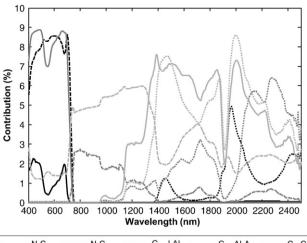
where the effects of LAI on canopy reflectance are rather limited, the SWIR is highly sensitive to LAI between 1000 nm and 1400 nm as illustrated by Fig. 3. This means that caution is advised when using these indexes for water retrieval.

The response of canopy reflectance to leaf optical properties was evaluated by Baret et al. (1994), who showed that leaf biochemical signals could be enhanced at the canopy level by up to a factor of two. All subsequent simulations using more rigorous statistical methods including the Design Of Experiments for Simulation method (DOES, Bacour et al., 2001, 2002b,c) or the Extended Fourier Amplitude Sensitivity Test (EFAST, Bowyer & Danson, 2004) have confirmed these results. Such methods make it possible to perform comprehensive sensitivity analyses of PROSAIL to identify, at any wavelength and/or in any direction, which variables explain most of the observed variability of a reflectance field. This gives valuable insight about the optimal wavebands (position, width) and/or viewing angles to retrieve the canopy biophysical variables.

For applications in imaging spectrometry, Bacour et al. (2002a) implemented the DOES method between 400 nm and 2500 nm to quantify the relative contributions of all canopy variables on reflectance, i.e., the percentage of the total variance explained by a given variable, and then to organize them into a hierarchy. The PROSAIL bidirectional reflectance factor was integrated over the hemisphere to provide a directional-hemispherical reflectance. As illustrated by Fig. 4, the results of this study indicate that chlorophyll content drives about 60% of the reflectance variation in the VIS, with a weaker contribution near 550 nm and 700 nm (the green and red edge regions which do not saturate at high concentrations). In the NIR, the most important variables are the average leaf angle and the leaf area index which contribute to reflectance in equal proportions. The SWIR confirms the prominent importance of light absorption by water with an average contribution of Cw of 50% between 1450 nm and 2100 nm. Surprisingly, this effect tends to lessen, and be replaced by LAI at wavelengths where the specific absorption coefficient of pure liquid water  $k_w$  is high (note that  $k_w \approx 30$  cm<sup>-1</sup> at 1450 nm,  $k_{\rm w} \approx 120~{\rm cm}^{-1}$  at 1950 nm, and  $k_{\rm w} \approx 90~{\rm cm}^{-1}$  at 2500 nm), which is also noticeable in Fig. 3. The ability to quantify interactions between variables is a major benefit of the DOES method. Interactions occur when the effect of variable A on a response depends on the level of variable B. The combined change in two variables may produce a



**Fig. 4.** Spectral variation of the contributions of the PROSAIL variables to the top-of-canopy directional–hemispherical reflectance. A Hyper Graeco Latin Geometric sampling scheme allowing full investigation of all interactions between two variables and consisting of 2401 simulations corresponding to different combinations of the PROSAIL input variables was used (adapted from Bacour et al., 2001, 2002a). Solar zenith angle  $\theta_3 = 31.6^\circ$ .

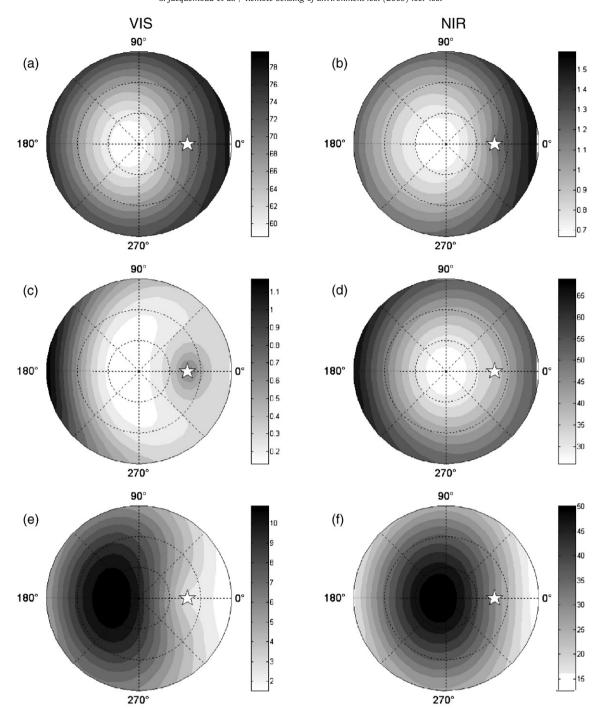




**Fig. 5.** Spectral variation of the contributions of interactions of the PROSAIL variables to top-of-canopy reflectance. Solar zenith angle  $\theta_s = 31.6^{\circ}$ .

greater effect than the sum of effects expected from either variable alone (Bacour et al., 2002c). Fig. 5 presents the nine most significant interactions between the canopy variables, considered two by two, over the twenty-one possible in their sampling scheme. In the VIS, the  $C_{\rm ab}$ -LAI and  $C_{\rm ab}$ -ALA interactions are each about 8%, while the LAI-ALA interaction prevails in the NIR with a contribution of 5–6%. The situation is more confused in the SWIR where predominant contributions vary between 3% and 7%, strongly depend on the wavelength and on leaf equivalent water thickness. The total contribution of the variables and their interactions almost equals 100%.

To investigate directional reflectance sensitivity, one can likewise compare a set of viewing angles which sample the whole hemisphere, at one waveband or over a given spectral domain (Bacour et al., 2001). The integrated 400-700 nm domain (VIS) and 700-900 nm domain (NIR) have been separated. In the VIS, results show that canopy reflectance is mostly influenced by  $C_{ab}$  in the backward direction where shadows are reduced (Fig. 6a). The negligible influence of chlorophyll in the NIR is expected and only explained by the selected wavelength range that includes the end of the red edge (Fig. 6b). For LAI, the forward directions seem to be favored in the VIS but with a very low contribution (Fig. 6c). The forward and backward directions where a large fraction of photons have interacted at least once with the canopy are to be preferred in the NIR (Fig. 6d), while near nadir observations when the soil background may be visible show the largest influence to leaf orientation characterized by an average leaf angle (Fig. 6f). The same trend is observed, to a lesser extent, in the VIS (Fig. 6e). For LAI, this means that the information carried by the reflectance of a turbid medium target viewed under a unique angle of 0° is poor compared to that measured at an oblique angle. Fig. 6 shows that the most accurate estimation of  $C_{ab}$ , LAI and ALA requires measurements at a minimum of three view angles: one in the forward direction, one at nadir, and one in the backward direction. Bowyer and Danson (2004), using a similar approach, also determined the spectral domain where canopy reflectance is the most sensitive to the leaf water content or to its mass per area. Indeed, by quantifying the contribution of each input variable to the model outputs, as well as their interactions, such analyses have been informative in isolating the optimal wavebands and viewing directions to retrieve canopy biophysical characteristics. Recently, Verhoef and Bach (2007) integrated PROSAIL with the Hapke soil BRDF model and an atmospheric radiative transfer model (see Fig. 2) to assess the performance of CHRIS (Compact High Resolution Imaging Spectrometer) onboard PROBA. They demonstrated that top-of-atmosphere S. Jacquemoud et al. / Remote Sensing of Environment xxx (2009) xxx-xxx



**Fig. 6.** Directional variation of the contribution (%) of the PROSAIL variables to the top-of-canopy reflectance: (a-b)  $C_{ab}$ , (c-d) LAI, and (e-f) ALA (adapted from Bacour et al., 2001). The solar zenith angle at  $\theta_s = 31.6^{\circ}$  is indicated by a star.

hyperspectral radiances under multiple view angles could be accurately predicted. These types of coupled vegetation-atmosphere sensitivity analyses are however scarce in the literature.

## 5. Validation of PROSPECT and SAIL models

Validation is an important issue that consists in assessing the quality of the model. This can be firstly achieved by comparing outputs with reflectance measurements at different scales. Most investigations that concentrated on PROSPECT and SAIL, separately, will not be detailed in this paper. In summary, the PROSPECT model proved to perform well on broadleaves and to provide a reasonable description of needle optical properties, even though the basic assumptions

associated with the plate model are obviously violated. Validation of the SAIL model was achieved by several authors based on experiments, mostly over crops where direct measurements of canopy structure are tractable. All reported relatively good agreement with observed data though the sampling of the variable space and the measurement configurations tested were limited. As for PROSAIL, direct comparisons of modeled and measured spectra were performed by Andrieu et al. (1997) and Danson and Aldakheel (2000) to monitor changes in spectral reflectance of a sugar beet crop caused by diurnal water stress. Verhoef and Bach (2007) tested the quality of 4SAIL2 and Schlerf et al. (2007) compared 4SAIL2 and FLIM, a hybrid model also coupled with PROSPECT, with CHRIS-PROBA satellite observations over broadleaf and conifer forest stands.

While such approaches show trends, they are not actual validations of the model because input variables have been tuned, or the available information is incomplete, which limits the evaluation process. To prevent such limitations, validation could be achieved by comparison with some reference radiative transfer model outputs when input variables are accurately known and can be manipulated easily. For instance, SAIL was compared with three-dimensional models of maize canopies (Weiss et al., 2000). And recently, the latest versions of SAIL were successfully compared to other 1-D and 3-D models for homogeneous canopies in the framework of the RAMI (RAdiation transfer Model Intercomparison) experiment, organized by the Joint Research Centre in Ispra, Italy (Widlowski et al., 2007). Model inversion process, as discussed in the following section, will provide a more comprehensive validation of PROSAIL.

### 6. Using PROSAIL to design and evaluate vegetation indexes

PROSAIL has been particularly useful in screening, designing and evaluating vegetation indexes: a query in the ISI Web of Science on 'SAIL' & 'VI' & 'vegetation' yields 8 papers. Among these, Clevers and Verhoef (1993), Plummer et al. (1994) and Chaurasia and Dadhwal (2004) verified the relationship between LAI and WDVI (Weighted Difference Vegetation Index), AVI (Angular Vegetation Index), and NDVI (Normalized Difference Vegetation Index), respectively, for varying leaf and canopy factors. Baret et al. (1995) compared eight vegetation indexes using a neural network approach to retrieve canopy gap fraction. Haboudane et al. (2002) and Zarco-Tejada et al. (2004b) simulated canopy reflectance spectra in the VIS-NIR to test the ratio of TCARI (Transformed Chlorophyll Absorption in Reflectance Index) to OSAVI (Optimized Soil-Adjusted Vegetation Index), which was expected to be sensitive at low chlorophyll values and resistant to nonphotosynthetic plant materials. In the SWIR, Zarco-Tejada et al. (2003) and Bowyer and Danson (2004) related the fuel moisture content at canopy level to SRWI (Simple Ratio Water Index) and NDWI (Normalized Difference Water Index), respectively. These two studies illustrated the difficulty in obtaining accurate estimates using semiempirical approaches and demonstrated the need for a coupled leafcanopy model to successfully estimate C<sub>w</sub> at the canopy level. Cheng et al. (2006) tested PROSPECT linked to different canopy models including SAIL to evaluate the impact of soil and canopy conditions on the retrieval of Cw. Within the same category, Broge and Leblanc (2000) and Le Maire et al. (2008) produced large reflectance datasets using PROSAIL to select and calibrate normalized reflectance difference indexes that are sensitive to leaf chlorophyll, dry matter content or LAI. The latter paper showed good agreement between field measurements and remote sensing estimates for these variables, from tree scale (ASD spectra) to regional scale (HYPERION images). Nonetheless, direct comparison of model-derived indexes with field measurements remains scarce.

## 7. Inversion of PROSAIL to retrieve canopy biophysical variables

The remote sensing inverse problem is critical when the radiometric signal has to be interpreted in terms of canopy biophysical characteristics. The inversion of PROSAIL gave rise to active research efforts and this success can be explained by the relatively small number of input variables required and good computer efficiency (Jacquemoud et al., 2000). A general description of the inverse theory, which is beyond the scope of this paper, can be found in Tarantola (2005). Its formulation for radiative transfer models devoted to exploit remote sensing observations was specified by Verstraete et al. (1996), Kimes et al. (2000), Liang (2003), and recently by Baret and Buis (2008) who reviewed the state of the art in this domain.

In brief, we may represent the mathematical model of a physical system, for instance PROSAIL, by the symbol m and the variables needed to completely describe the system by the symbol x. The

physical observation, here the reflectance *R*, is formally expressed by:

$$R = m(x) + \varepsilon \tag{1}$$

Eq. (1) is a short notation for the set of equations  $R_i = m_i(x_1x_2,...x_k) + \varepsilon_i$  for (i=1,2...n).  $\varepsilon_i$  represents the residual errors between simulated and measured reflectance. If some variables listed in Table 1 are perfectly known, e.g. the zenith and azimuth angles, they can be considered as fixed constants. If they are uncertain, e.g. the canopy biophysical characteristics, they must enter the parameter set x. The inverse problem of a nonlinear model such as PROSAIL is based on the minimization of a cost (or misfit) function  $\delta^2$  that concurrently measures the discrepancies between i) the observed and simulated reflectance and ii) the variables to estimate and the associated prior information:

$$\delta^{2} = \sum_{i=1}^{n} \left( \frac{R_{i} - m_{i}(x_{1}, x_{2}, \dots, x_{k})}{\sigma_{Ri}} \right)^{2} + \sum_{j=1}^{k} \left( \frac{x_{j} - x_{j}^{\text{prior}}}{\sigma_{xj}} \right)^{2}$$
 (2)

where  $\sigma_{Ri}$  and  $\sigma_{xj}$  are respectively the diagonal elements of the error covariance matrices on observations and parameters.  $\sigma_{Ri}$  corresponds to the measurement/model uncertainties and  $\sigma_{xi}$  to the uncertainty of any prior information on the variables to estimate  $x_j^{\text{prior}}$ , i.e., obtained independently of the measurements. If statistics  $\sigma_{Ri}$  and  $\sigma_{xi}$  are not available, the cost function simplifies while increasing the risk of converging towards local minima due to the non-unicity of the inverse solution. Eq. (2) does not incorporate boundary constraints or relationships between parameters. Two main categories of inversion approaches have been exploited: the first one emphasizes the first part of the misfit function such that the solution corresponds to a minimum distance between reflectance measurements and model simulations, with respect to the a priori constraints. Iterative optimization, Markov chain Monte Carlo methods and look-up tables belong to this category. The other family of approaches emphasizes the second part of the misfit function, focusing on the space of canopy biophysical variables: a parametric model is adjusted over the surface response between reflectance and the biophysical variables of interest. VIs related to the biophysical variables through parametric models and artificial neural networks belong to this second category.

### 7.1. Approaches based on the observation space

These approaches were the first to be applied to canopy reflectance model inversion. Goel and Strebel (1983) foresaw the potential use of canopy reflectance models for estimating agronomic variables, at a period when models were still in their infancy, and explored the inversion of the Suits model (Suits, 1972), the forerunner of SAIL, and then of the SAIL model (see Goel, 1989). Various iterative minimization techniques have been implemented (e.g., simplex, steepest descent, quasi-Newton, genetic algorithms) that mainly differ from the downhill search algorithms, the capacity to avoid trapping in local minima, and constraints on the range of variation of each unknown variable to be estimated. The number of variables to be concurrently adjusted and the number of configurations considered define the size of the inverse problem. As pointed out by Jacquemoud et al. (1994), it is somewhat difficult to make general recommendations as to the choice of one algorithm instead of another because these are typically well-adapted to the problem being considered. Jacquemoud and Baret (1993) made the first attempt to jointly estimate biochemical and structural attributes of plant canopies (namely  $C_{ab}$ ,  $C_{w}$ , and LAI) from high resolution reflectance spectra acquired at nadir in the solar domain on sugar beet crops with the simplex minimization algorithm. As above-mentioned, inverting the SAIL model wavelength per wavelength is a highly underdetermined problem because three unknowns have to be estimated at each wavelength in addition to

canopy structure variables: leaf reflectance, transmittance, and soil reflectance. Coupling SAIL with PROSPECT offers therefore a unique advantage of imposing a strong spectral constraint on the inversion process that decreases drastically the number of unknown variables while providing enhanced spectral consistency. However, some inversion instabilities were observed due to compensations between several canopy variables (e.g., LAI and LIDF) in the inversion process (Jacquemoud, 1993; Jacquemoud et al., 1995, 2000; Zarco-Tejada et al., 2001; Zhang et al., 2005) when using actual AVIRIS (Advanced Visible Infrared Imaging Spectrometer), CASI (Compact Airborne Spectrographic Imager), TM (Thematic Mapper) or MODIS (Moderate Resolution Imaging Spectroradiometer) observations, or even synthetic reflectance data (Weiss et al., 2000). These studies showed increased robustness and accuracy when estimates of biochemical contents were integrated at the canopy level (total chlorophyll,  $C_{ab} \times LAI$ , or water,  $C_w \times LAI$ ) rather than at the leaf level (Jacquemoud et al., 1994; Weiss et al., 2000). An optimized number of wavebands and view angles, carefully selected, however, should permit more reliable separation of the variables (Bacour et al., 2002b; Meroni et al., 2004). Nevertheless, radiative transfer model inversion is generally ill-posed because of measurement and model uncertainties, and the often underdetermined nature of the problem since the radiometric signal carries only limited information (Combal et al., 2002a,b; Baret & Buis, 2008). Regularization of the inversion problem to get more stable and accurate solutions requires introducing prior information on the distribution of the variables, as well as possible additional spatial or temporal constraints (Koetz et al., 2005; Lauvernet et al., 2008).

Although iterative minimization methods proved to be efficient for case studies or limited number of observations to be processed, they could not be applied over large spatial or temporal domains because of prohibitive computation times. Operational implementation of such methods is facilitated when using pre-computed simulated data bases. Look-up tables are a simple technique that consists of generating a training table with the model for a discrete set of input variables covering their prescribed range of variation. They offer the advantage of providing the global minimum if the variable space is sufficiently sampled, avoiding the tricky problem of local minima. Sensitivity analyses of the model can help to better choose the subdomains where reflectance is sensitive to a variable, when all of them are varying; and as in the case of iterative methods, prior information can be introduced. Implementations of this method permitted estimation of Cab, LAI, fAPAR, and fCover (Weiss et al., 2000; Combal et al., 2002a; Verhoef & Bach, 2003a; Koetz et al., 2005; González-Sanpedro et al., 2008).

## 7.2. Approaches focusing on the space of canopy variables

Although the use of vegetation indexes may be considered as an inverse technique when radiative transfer models are used to calibrate parametric equations between VIs and some canopy characteristics, this will not be discussed in this section since it has already been addressed. Machine learning techniques such as artificial neural networks also belong to this type of approaches and have lately become a popular method to operationally invert models because of their high computational speed, once they have been calibrated. They interconnect a set of inputs (the reflectances) to a set of outputs (the canopy biophysical variables), assuming that they are functionally related, during the so-called "learning phase". Their performances mainly depend on the characteristics of the training database, for which no explicit assumption about the physics of radiative transfer within plant canopies is mandatory, so that pairs of reflectance observations and corresponding biophysical variables can be used, in theory, to train an artificial neural network. However, because such datasets gathering both radiometric and biophysical data are scarce and prone to significant uncertainties associated to ground measurements of canopy characteristics, observations are conveniently replaced by model simulations. This approach has been successfully applied to VEGETATION (Weiss & Baret, 1999), airborne POLDER (POLarization and Directionality of the Earth's Reflectances, Weiss et al., 2002), Landsat TM (Atzberger, 2004), and MERIS (Medium Resolution Imaging Spectrometer, Bacour et al., 2006) to determine LAI, gap fraction, fAPAR, or the canopy chlorophyll content. Trombetti et al. (2008) recently published the first monthly global maps of vegetation canopy water content (LAI  $\times$   $C_{\rm w}$ ) over the continental USA using MODIS data trained with an artificial neural net.

A frequently asked question is "which method should be selected to solve an inversion problem?". The answer varies because each approach has specific advantages and disadvantages. The performance of iterative methods, look-up tables, and artificial neural networks were compared using synthetic datasets by Combal et al. (2002b). While results demonstrated a significant improvement of the retrieval when using prior information, the accuracy seemed to depend in a large manner on model uncertainties. For example, SAIL may not represent properly the structure of heterogeneous plant canopies that deviate from the model hypotheses. The accuracy also depends on measurement errors associated with the signal-to-noise ratio of the sensor and on the quality of the calibration procedure, i.e., mostly the removal of the atmospheric effects. Prior information on model variables is represented by a probability distribution that is often empirically characterized because of a lack of observations on vegetation canopies corresponding to different plant species and ecosystems, or because the available information is incomplete and scattered throughout the literature. Collecting databases on leaf biochemistry to better document the range of variation and probability density functions of  $C_{ab}$ ,  $C_{w}$ , and  $C_{m}$ , for instance, would significantly improve the mapping of these constituents for applications in both agriculture and ecology. The next section emphasizes some of these applications.

## 8. Application of PROSAIL

Table 2 summarizes some examples of application of PROSAIL for canopy biophysical variables estimation. It shows that most of the studies are focused on the spectral dimension of observations. Directional observations mainly stem from airborne and spaceborne POLDER instruments. Even when directional observations are available (e.g., multi-temporal VEGETATION images), researchers seem to prefer to fit a parametric BRDF model and then use normalized reflectances such as the one at nadir viewing as input. Although interrogation of ISI Web of Science shows 22 articles dealing with 'SAIL' & 'directions', most of these papers are related to improvement of the modeling of directional effects, or on theoretical considerations on optimal sampling of directions. Association of 'SAIL model' & 'hyperspectral' or 'imaging spectroscopy data' yield only 11 articles, all published after 2001. Association between 'PROSPECT' & 'hyperspectral' provides 24 articles published after 2000 while association with 'imaging spectroscopy' yields 5 articles published before 2000, showing a possible trend in terminology, 'hyperspectral' replacing 'imaging spectroscopy'.

Because of the basic physical assumptions made in PROSPECT and SAIL (e.g., Lambertian broad-flat leaves, semi-infinite horizontally homogeneous plant canopies), and because it represents compromises that have generally been considered acceptable, PROSAIL was first used with crops for applications in agriculture as illustrated by Table 2. In addition, the biophysical characteristics of crops are easier to measure than those of other vegetation types such as forests. SAIL and PROSPECT are now operationally used in precision farming, an economically profitable concept which also preserves the environment. In this concept, intra-field variability is identified so that the appropriate agricultural inputs (fertilizers, fungicides, herbicides, etc.) are only applied at specific locations and cultural practices are

**Table 2**Examples of studies on canopy biophysical variables estimated by inversion of PROSAIL for applications in agriculture, forestry, environment or ecology.

Sensor	VIS	NIR	SWIR	$N_{\rm v}$	Plant species	Variable	Method	Reference
Ground data								
CIMEL/CROPSCAN	1-6	1-2		1	Sugar beet	Gap fraction	NNT	Baret et al. (1995)
GER IRIS Mk IV	3-30	1-60	2-90	1	Sugar beet	$C_{\rm ab}$ , $C_{\rm w}$ , LAI	OPT	Jacquemoud et al. (1995)
GER IRIS Mk IV	7	4		1	Sugar beet	$N$ , $C_{ab}$ , $C_{w}$ , LAI, ALA, $s_{L}$	LUT	Combal et al. (2002a)
GER 1500	30	50	61	1	Potato	LAI, ALA	OPT	Casa & Jones (2004)
ASD	300	600	900	1	New Guinea impatiens	N, C <sub>w</sub> , LAI, ALA	OPT	Yang & Ling (2004)
ASD	300	600	900	1	Beech, oak	$C_{\rm ab}$ , $C_{\rm m}$ , LAI	VI	Le Maire et al. (2008)
Airborne data								
CAESAR	2	1		2	Onion, pea, potato, sugar beet, wheat	N, $C_{ab}$ , LAI, ALA, $s_L$	OPT	Jacquemoud et al. (1994)
CASI	7	3		1	Maize, soybean	$C_{\mathrm{ab}}$ , LAI	OPT	Jacquemoud et al. (2000)
POLDER	3	1		var	Alfalfa, maize, sunflower, wheat	$C_{\rm ab}$ , LAI, ALA, $s_{\rm L}$ , $lpha_{\rm soil}$	OPT	Bacour et al. (2002b)
POLDER	3	1		var	Alfalfa, maize, sunflower, wheat	Gap fraction, LAI	NNT	Weiss et al. (2002)
CASI	7	4		1	Maize	LAI	LUT	Koetz et al. (2005)
CASI	40	32		1	Sugar mapple	$C_{\rm ab}$ , LAI	VI	Zarco-Tejada et al. (2001)
DAIS	20	10	6	1	Poplar	LAI	OPT	Meroni et al. (2004)
ROSIS/DAIS	40	32		1	Olive trees	C <sub>ab</sub> , LAI	VI	Zarco-Tejada et al. (2004b)
Spaceborne data								
MODIS	3	2	2	1	Chaparral	$C_{w}$	OPT	Zarco-Tejada et al. (2003)
POLDER	2	1		11	Global domain	LAI	NNT	Lacaze (2005)
MODIS	3	2	2	1	Black birch, red oak, red mapple, white pine	$N$ , $C_{ab}$ , $C_{w}$ , $C_{m}$ , $C_{b}$ , PAI, $f$ Cover	MCMC	Zhang et al. (2005)
MERIS	7	4		1	Global domain	$LAI \times C_{ab}$ , LAI, fAPAR, fCover	NNT	Bacour et al. (2006)
IKONOS, SPOT, ETM+	2-3	1	0-2	1	Temperate coniferous and deciduous forest	LAI	VI	Soudani et al. (2006)
MODIS	3	2	2	1	Vegetation of the continental USA	$LAI \times C_w$	NNT	Trombetti et al. (2008)
VEGETATION	2	2		1	Global domain	LAI, fAPAR, fCover	NNT	Baret et al. (2007), Weiss et al. (2007)
TM, TM+	3	1	1	1	Corn, sugar beet, potato, sunflower, alfalfa, garlic, onion, other	LAI	LUT	González-Sanpedro et al. (2008)
HYPERION	34	50	136	1	Broad-leaved forest	C <sub>ab</sub> , C <sub>m</sub> , LAI	VI	Le Maire et al. (2008)

Sensors used, number of bands available per spectral domain (VIS, NIR, SWIR), number of view directions ( $N_v$ ), plant species, inferred canopy variables and inverse method (OPT: iterative minimization; VI: vegetation index; LUT: look-up table; MCMC: Markov chain Monte Carlo; NNT: artificial neural network) along with the corresponding references are indicated.

modulated depending on canopy actual status as seen from remote sensing. For instance, the crop monitoring service of Infoterra (http://www.infoterra.fr/) called FarmStar, includes the physics of PROSAIL. It uses both satellite and airborne data on an operational basis to provide timely field-level maps of LAI and nitrogen recommendation, assuming that there is a strong relationship between nitrogen and chlorophyll content (Blondlot et al., 2005).

The area of applications of PROSAIL is meanwhile extended to natural vegetation canopies although they may not meet all requirements of the model. Broadleaf homogeneous canopies are indeed seldom encountered in nature and are a rather idealized approximation for many ecosystems. However, since an exhaustive description of the 3-D structure of most terrestrial ecosystems is impossible with our present tools, the simplified assumption that considers horizontal homogeneity should not invalidate the use of 1-D models. Table 2 mainly shows large-scale ecosystem studies based on medium resolution spaceborne sensors such as MODIS, MERIS, VEGETATION, and POLDER for the estimation of global fields of LAI, fCover, fAPAR,  $LAI \times C_{ab}$  or  $LAI \times C_{w}$ . Validation using ground measurements is a difficult task at this scale (Morisette et al., 2006) but results obtained by Bacour et al. (2006) and Weiss et al. (2007) show that estimates of fAPAR are reliable and accurate, while those of LAI suffer from saturation effects that cannot be dissociated from radiative transfer within plant canopies. The retrieved LAI values appear thus closer to an effective LAI value, that may partly explain the early saturation observed on LAI products. Nevertheless, as compared to LAI products collection 4 derived from MODIS through inversion of 3-D radiative transfer models (Myneni et al., 2002), PROSAIL LAI products derived from VEGETATION sensors appear to perform reasonably well when compared with effective LAI derived from gap fraction measurements performed at the ground level (RMSE = 0.73). On forest canopies, PROSAIL LAI derived from HYPERION sensors (using wavelengths at 970 and 1725 nm) showed only a slight saturation (values as high as 10 were easily obtained), and a higher RMSE was observed (RMSE = 1.56 for LAI ranging from 0 to 10).

Inspection of the distribution of subject categories addressed in articles dealing with SAIL or PROSPECT models (Table 3) shows here again a close parallelism between scores by SAIL and PROSPECT. When focusing on SAIL, 'remote sensing' and 'imaging science' get non surprisingly the highest scores, just before 'environmental sciences'. Then, 'agronomy' and 'meteorology and atmospheric sciences' correspond to the main application, getting significantly higher scores than, 'forestry', 'ecology' and 'agriculture multidisciplinary'. This confirms the previous comments extracted from Table 2 on the application domains.

Table 3
Distribution (in %) between subject categories for articles using PROSPECT ('PROSPECT' & 'leaf') and SAIL ('SAIL' & 'reflectance') as extracted from ISI Web of Science.

Subject category	PROSPECT	SAIL
Remote sensing	29	29
Imaging science and photographic technology	27	27
Environmental sciences	25	23
Agronomy	5	5
Plant sciences	3	0
Geochemistry and geophysics	2	1
Geosciences multidisciplinary	2	2
Engineering, electrical and electronic	2	1
Meteorology and atmospheric sciences	2	4
Forestry	1	2
Horticulture	1	0
Water resources	1	0
Ecology	0	2
Agriculture, multidisciplinary	0	2
Engineering, aerospace	0	1
Geography, physical	0	1
Total	100	100

Note that one article could address several subject categories.

### 9. Conclusion

The coupling of PROSPECT with SAIL models made it possible to physically interpret spectral and directional reflectance fields as sampled by Earth observation sensors in terms of leaf biochemical contents and canopy architecture. When run in direct mode, PROSAIL provides a means to generate databases and test new spectral indexes, and to perform sensitivity analyses that will allow better designs on forthcoming sensors devoted to specific applications, long before their launch. When embedded in an inversion procedure, PROSAIL turns into a powerful tool to derive new products. The first large scale maps of chlorophyll content appeared just a few years ago, those of water content and dry matter content (or specific leaf area) a few months ago. In the future, the functionality of terrestrial ecosystems could be monitored in a totally different way when estimating the main leaf pigments individually, e.g. chlorophylls and carotenoids, when interpreting the xanthophyll cycle and fluorescence emission fluxes in green leaves in terms of photosynthesis efficiency, and when the UV-screening role of anthocyanins in plant foliage is fully understood. The mapping of vegetation water content is another emerging application for forest fire risk assessment, and forest defoliation resulting from heat waves, insect or fungus infections. This obviously goes through new developments and evolution of these models, to get more detailed and realistic simulations of canopy reflectance with inclusion of additional processes such as fluorescence or thermal infrared emission, which are already ongoing (Miller et al., 2005; Zarco-Tejada et al., 2006; Verhoef et al., 2007).

Although other models have been developed, generally they have received less validation and comparison to previously existing ones, either due to lack of resources or limited access by other researchers. The large diffusion of PROSPECT and SAIL in the research community is attributed to their simplicity, accuracy and, above all, their availability. These two models, individually or together, have probably contributed to pave the road towards improved use of our physical understanding of radiative transfer processes in plant canopies. However, they are still often perceived as excessively complicated tools compared to vegetation indexes. The inversion of PROSAIL and of the other available codes, is actually still a job for a specialist. The design of optimized vegetation indexes that include aspects of the physics of the radiative transfer within plant canopies is destined for success. Online educational tools like the Graphical User Interfaces (GUI) which allow people to "play" with models would be very helpful to make users understand their operation and to recognize their value in obtaining more accurate information about plant biophysical

As reviewed in this paper, plant canopy reflectance models have become essential tools for the analysis of optical remote sensing data, providing meaningful links between radiometry and environmental applications, such as ecological processes, environment and precision agriculture. Radiative transfer models are now routinely used by space agencies or more specific service providers to produce spatially and temporally continuous fields of canopy biophysical variables to be integrated into process models for decision making. Desirable biophysical variables required by these process models are fAPAR, LAI, leaf nitrogen content, leaf mass per area, stand biomass, leaf biomass, etc. (Plummer, 2000; Le Maire et al., 2005; Davi et al., 2006). However, the SAIL model has intrinsic limitations in its capacity to simulate heterogeneous canopies showing clumping at several scales which explains why, under these circumstances, use of RT models to estimate some canopy characteristics finally achieve performances often comparable to those of empirical relationships with vegetation indexes. Improvements will require a more complex description of canopy architecture to account for leaf clumping as already initiated with hybrid turbid/geometrical models. Unfortunately, these improvements will require additional variables that may vary with time and space, needing them to be therefore estimated. A good balance is thus mandatory between realism and complexity for application through radiative transfer model inversion. Part of the increased complexity could be compensated for by exploiting prior knowledge on the distribution of variables, which will be much easier to define at relatively high spatial resolution (5–20 m) where most pixels will be 'pure', corresponding to only one type of vegetation. There are good times ahead for models!

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S. Jacquemoud et al. / Remote Sensing of Environment xxx (2009) xxx-xxx

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