Inversion of Monte Carlo Model for Estimating Vegetation Canopy Parameters

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The Monte Carlo technique for estimating model parameters is presented. The bidirectional reflectance factor is calculated by the Monte Carlo method of solving the integral equation of radiation transfer in plant canopies. A general inversion technique for the estimation of canopy parameters is considered. The method of calculating derivatives of the bidirectional reflectance factor with respect to unknown parameters using the same photon trajectories as in the solution of the direct problem is developed. The leaf dimensions are taken into account using a new extinction coefficient. Finally, numerical results for estimating three optical canopy parameters (coefficients of leaf reflectance, transmittance, and soil albedo) and four geometrical canopy parameters (leaf area index, two parameters of leaf angle distribution function, and leaf size parameter) are briefly discussed.

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INTRODUCTION

In recent years the development of remote sensing technology has made it increasingly important to investigate different algorithms for the solution of inverse problems. To solve the inverse problem means to be able to estimate the optical and geometrical parameters of leaf canopies from data of canopy reflectance.

Canopy reflectance models play a key role in the solution of this problem. Comprehensive reviews of the existing models have been presented by Goel (1988) and Myneni et al. (1989). There are two different types of models for describing the radiative regime of plant canopies: 1) geometrical models, where the canopy is simulated as geometrical objects of prescribed shapes, dimensions, and optical properties; 2) turbid medium models, where elements of the vegetation are treated as small absorbing and scattering particles with given optical properties, distributed randomly in horizontal layers, and oriented in given directions (Goel, 1988). The first type of models correspond more to sparse and heterogeneous canopies, and the second type is more applicable to denser and horizontally uniform canopies in which the vegetation elements are smaller in comparison to the height of the canopy (Ross, 1981). There exist as well hybrid models that take into account the dimensions of leaves in the framework of the turbid medium models (Nilson and Kuusk, 1989; Marshak, 1989; Myneni et al., 1990). One of these models was used by Antyufeev and Marshak (1990) for the calculation of canopy reflectance by the Monte Carlo method.

The first works devoted to the inverse problems for plant canopies are due to Goel and his colleagues (Goel, 1988 and references therein). They succeeded in solving the inverse problems for different models for both homogeneous and heterogeneous canopies. Their technique considered the minimization of the functional

$$F = \sum_i w_i [y_i - y_i']^2,$$

where y_i is the intensity calculated using a canopy reflectance model and y_i' is the intensity measured with some accuracy. Marshak (1987), using the technique developed for estimating parameters of the atmosphere from satellite data (Marchuk et al., 1980), could determine the optical parameters of the leaf canopy, using the Monte Carlo model of Ross and Marshak (1988; 1989). Nilson and Kuusk (1989) were able to invert their model by including "punishment functions" (that do not allow the estimated parameters to get "nonphysical" values) for the minimization of functional F. The inverse procedure was applied simultaneously to two sets of the optical parameters (in visible and near-infrared spectral regions) and to one set of geometrical parameters.

The purpose of the present paper is to show the invertibility of the Monte Carlo canopy reflectance model proposed by Antyufeev and Marshak (1990). The canopy reflectance model is based on the integral equation describing the radiative transfer process in a turbid plate medium. To consider the finite dimensions of the scattering centers, a new extinction coefficient was introduced. This coefficient depends additionally on the previous direction of photon travel (Marshak, 1989). In spite of the more complicated nature of the extinction and scattering coefficients (Myneni et al., 1990), this model can be considered as a first approximation for radiative transfer theory that includes the finite dimensions of leaves. The integral equation was solved by the Monte Carlo method, which allows us to follow the dependence of a photon on its previous history. In the present paper we attempt to develop a general Monte Carlo technique for estimating canopy parameters. It is necessary to emphasize that the derivatives with respect to the unknown parameters are calculated by the Monte Carlo method as well, using the same photon trajectories as for calculating the bidirectional reflectance factor (BDRF).

A brief outline of the paper is as follows: at first, we set up the problem (next section) and describe the algorithm for the solution of the inverse problem (third section). Then, for better understanding, we briefly summarize the reflectance model (fourth section). In the fifth section we develop the theory of calculating the derivatives. The "weight" factors for its calculation are presented as well. Some numerical results are provided in the sixth section.

STATEMENT OF THE PROBLEM

We shall use the notation in the recent papers of Marshak (1989) and Antyufeev and Marshak (1990). Let the point $x \sim (t, \mathbf{\Omega})$ be the point of phase space $X = [0, H] \otimes 4\pi$, where $H = t(T)$ is the leaf area index (LAI) of the canopy with a physical depth of T. Here, $t = t(z)$ is the cumulative leaf area index at depth z, and $\mathbf{\Omega} \sim (\mu, \phi)$ is the direction of photon travel before interaction. The vector $\mathbf{\Omega}_0 \sim (\mu_0, \phi_0)$, $\mu_0 < 0$ and $\mathbf{\Omega}^* \sim (\mu^*, \phi^*)$, $\mu^* > 0$ denote the directions of direct solar radiation and view, respectively. The random vector $\mathbf{\Omega}_L \sim (\mu_L, \phi_L)$, $\mu_L > 0$ is the leaf surface normal (directed away from its upper face). The optical depth from point z to the upper canopy boundary in the direction $\mathbf{\Omega}$ is defined as $\tau(x) = t(z)G(\mathbf{\Omega})$, where (Ross, 1981)

$$G(\mathbf{\Omega}) = \frac{1}{2\pi} \int_{\{2\pi^+\}} g_L(\mathbf{\Omega}_L) |\mathbf{\Omega} \cdot \mathbf{\Omega}_L| \, d\mathbf{\Omega}_L, \quad (1)$$

is the mean projection of leaf normals on direction $\mathbf{\Omega}$. In case of vertically homogeneous canopies and nondimensional leaves, the function $G(\mathbf{\Omega})$ plays the role of the extinction coefficient for the appropriate transport equation (Shultis and Myneni, 1988). Function $(2\pi)^{-1} g(\mathbf{\Omega}_L)$ is the leaf-normal probability density. We assume for simplification that the leaf normals are uniformly distributed with respect to azimuth ϕ_L, i.e.,

$$\frac{1}{2\pi} g_L(\mathbf{\Omega}_L) = \frac{1}{2\pi} g_\theta(\theta_L),$$

where $1/2\pi$ is the azimuthal density and g_θ is the probability density with respect to the polar angle θ_L ($\mu_L = \cos\theta_L$). We propose a simple trigonometrical model (Bunnik, 1978)

$$g_\theta(\theta_L)\, d\mathbf{\Omega}_L = 2/\pi[1 + b\cos 2\theta_L + c\cos 4\theta_L]\, d\theta_L\, d\phi_L$$

The parameters b and c define the polar leaf angle distribution. The first parameter $a = 1$ is fixed, which follows from the normalization

$$\frac{1}{2\pi}\int_{\{2\pi^+\}} g_L(\mathbf{\Omega}_L)\, d\mathbf{\Omega}_L = 1.$$

The signs $\{4\pi\}$, $\{2\pi^+\}$, and $\{2\pi^-\}$ denote that the integrals are over the whole unit sphere, upper and lower hemispheres, respectively.

The next parameter, κ, characterizing the dimension of scattering centers (leaves), follows from the papers by Nilson and Kuusk (1989), Marshak (1989), and Antyufeev and Marshak (1990). Namely, the new extinction coefficient that accounts for the hot-spot effect in a simple way is

$$\sigma_\kappa(t,\mathbf{\Omega}',\mathbf{\Omega}) = \begin{cases} G(\mathbf{\Omega}), & \mu\mu' > 0, \\ G(\mathbf{\Omega})h_\kappa(t,\mathbf{\Omega}',\mathbf{\Omega}), & \mu\mu' < 0. \end{cases} \quad (2)$$

where

$$h_\kappa(t,\mathbf{\Omega}',\mathbf{\Omega}) = 1 - \left[\frac{G(\mathbf{\Omega}')|\mu|}{G(\mathbf{\Omega})|\mu'|}\right]^{1/2} \times \exp\left[-\frac{\Delta(\mathbf{\Omega},\mathbf{\Omega}')t}{\kappa H}\right],$$

$$\Delta(\mathbf{\Omega},\mathbf{\Omega}') = \left(\mu^{-2} + \mu'^{-2} + 2(\mathbf{\Omega}'\cdot\mathbf{\Omega})/|\mu\mu'|\right)^{1/2}.$$

The expression (2) allows us to take into account the leaf sizes only for those photons that are redirected into the retrohemisphere interaction ($\mu\mu' < 0$). For those photons that travel "forward" ($\mu\mu' > 0$), the extinction coefficient (1) is unchanged. In case of retroscattering (reflectance)

$$\mathbf{\Omega} = -\mathbf{\Omega}', \quad \Delta(-\mathbf{\Omega}',\mathbf{\Omega}') \equiv 0, \quad \sigma_\kappa \equiv 0$$

and the photon goes back unweakened. In order to exclude the extreme cases, where $\sigma_\kappa < 0$ (for example, the photon travels parallel to the vertical leaves, i.e., $G(\mathbf{\Omega}) = (2/\pi)(1-\mu^2)^{1/2}$ and $|\mu| = 1$), it is assumed that

$$\left[\frac{G(\mathbf{\Omega})|\mu'|}{G(\mathbf{\Omega}')|\mu|}\right]^{1/2} \geqslant \exp\left[-\frac{\Delta(\mathbf{\Omega},\mathbf{\Omega}')t}{\kappa H}\right],$$

and $h_\kappa = 0$ in the opposite case. The detailed theory of the radiative transfer in leaf canopies with finite dimensional scattering centers can be found in the paper of Myneni et al. (1990).

We introduce the area scattering transfer function $P(\mathbf{\Omega}' \to \mathbf{\Omega})$ as (Shultis and Myneni, 1988),

$$P(\mathbf{\Omega}' \to \mathbf{\Omega}) = \frac{1}{2\pi}\int_{\{2\pi^+\}} g_L(\mathbf{\Omega}_L)|\mathbf{\Omega}'\cdot\mathbf{\Omega}_L| \times f(\mathbf{\Omega}_L;\mathbf{\Omega}' \to \mathbf{\Omega})\, d\mathbf{\Omega}_L / G(\mathbf{\Omega}'), \quad (3)$$

where the leaf phase function $f(\mathbf{\Omega}_L;\mathbf{\Omega}' \to \mathbf{\Omega})$ in the simplest case of a bi-Lambertian leaf surface with diffuse reflectance coefficient r_L and diffuse transmittance coefficient t_L can be written as

$$f(\mathbf{\Omega}_L;\mathbf{\Omega}' \to \mathbf{\Omega}) = \begin{cases} r_L|\mathbf{\Omega}\cdot\mathbf{\Omega}_L|/\pi, \\ (\mathbf{\Omega}\cdot\mathbf{\Omega}_L)(\mathbf{\Omega}'\cdot\mathbf{\Omega}_L) < 0, \\ t_L|\mathbf{\Omega}\cdot\mathbf{\Omega}_L|/\pi, \\ (\mathbf{\Omega}\cdot\mathbf{\Omega}_L)(\mathbf{\Omega}'\cdot\mathbf{\Omega}_L) > 0. \end{cases} \quad (4)$$

Let the soil surface be Lambertian as well and be characterized by its albedo r_s.

So, our model describes the plant canopy and reflectance from the soil surface by seven parameters $(b, c, \kappa, H, r_L, t_L, r_s)$. Now we can set the problem as follows. Both the monodirectional solar and diffuse sky radiation illuminate the plane parallel layer of vertically homogeneous leaf canopy. There are detectors above the canopy that measure the BDRF $R(\mathbf{\Omega}^*)$ in the direction $\mathbf{\Omega}^*$. Knowing the function R, the problem is to obtain information on the three optical parameters (r_L, t_L, and r_s) and four geometrical parameters (b, c, κ, and H), or, in other words, we need to solve the inverse problem of estimating the medium parameters from the reflection data. The more important parameters are the geometrical parameters since it is more difficult to measure them in field experiments.

MATHEMATICAL APPROACH

The transport equation includes the desired parameters in a quite complicated way, since it is difficult, or for some parameters impossible, to derive a closed system of analytical equations. Moreover, such experiments lead us to different equations for different parameters. It is far more convenient to use a sufficiently universal algorithm.

Here we shall use a modification of the Newton method (Kantorovich and Akilov, 1978). Let $\alpha_1^*, \ldots, \alpha_n^*$ be the desired values of n parameters $\alpha_1, \ldots, \alpha_n$ that we need to estimate. Denote the BDRF for the canopy with parameters $\alpha_1, \ldots, \alpha_n$ in the view direction $\mathbf{\Omega}^*$ by

$$R_k \equiv R_k(\alpha_1, \ldots, \alpha_n), \quad k = 1, \ldots, N \geqslant n.$$

Let

$$R_k^* \equiv R_k^*(\alpha_1^*, \ldots, \alpha_n^*)$$

be the measured BDRF. So, for the estimation of the parameters $\alpha_1^*, \ldots, \alpha_n^*$, we consider the system of nonlinear equations

$$R_k(\alpha_1, \ldots, \alpha_n) = R_k^*, \quad k = 1, \ldots, N, \qquad (5)$$

where R_k is a function of sufficiently complicated nature. We shall solve the system (5) by the Newton–Kantorovich method (this is also known as Newton–Raphson method),

$$\alpha_i^{l+1} = \alpha_i^l + \delta_i^l, \quad i = 1, \ldots, n, \quad l = 0, 1, \ldots, \qquad (6)$$

where δ_i^l satisfy the system of linear equations,

$$\sum_{i=1}^{n} \frac{\partial R_k}{\partial \alpha_i} \delta_i^l = R_k^* - R_k(\alpha_1^l, \ldots, \alpha_n^l), \quad k = 1, \ldots, N \qquad (7)$$

with iteration index l. The initial approximation in the iterative process (6) is taken to be the set of parameters $\alpha_1^0, \ldots, \alpha_n^0$, the elements of which are a guess for values of desired parameters. The iterative process is stopped if

$$|R_k^* - R_k(\alpha_1^l, \ldots, \alpha_n^l)| < \varepsilon,$$

where $\varepsilon > 0$ is a given small number.

The system (7) is overdefined. The simplest way to solve it is to multiply both sides of (7) by the matrix adjoint to the matrix $\{\partial R_k / \partial \alpha_i\}$, i.e., to use a least square method. However, the system so obtained may be highly unstable and it is necessary to use regularization theory (Baltes, 1980). We use the Monte Carlo method for calculation of both the BDRF R_k (next section) and its derivatives $\{\partial R_k / \partial \alpha_i\}$ (section after next).

Sometimes it is very useful to modify the above scheme. Let us introduce the BDRF by two addents $R = R_1 + (R - R_1)$, where R_1 is the contribution to the BDRF of the first-order scattering photons. One notices that this contribution is quiet large for many practically important cases (for instance, in the spectral region of photosynthetically active radiation). It is not difficult to check that the same conclusion is valid for the corresponding derivatives as well. Then it is natural to try to change the derivatives $\partial R / \partial \alpha$ to the derivatives $\partial R_1 / \partial \alpha$ in system (7). The advantage of such a change is connected with the calculation of derivatives (section after next). The calculation of $\partial R / \partial \alpha$ with satisfactory accuracy demands significant computer time. On the other hand, the calculation of derivatives $\partial R_1 / \partial \alpha$ is carried out in parallel with the calculation of the corresponding BDRF (the same photon trajectories are used) and does not require significant extra computer time. Of course, the theoretical rate of convergence of the iterative process (6)–(7) becomes slower; however, it can be compensated by the more accurate calculation of the derivatives $\partial R_1 / \partial \alpha$. Moreover, the relative difference between $\partial R_1 / \partial \alpha$ and $\partial R / \partial \alpha$ is not large for small values of leaf area index. It allows us to use the derivatives $\partial R_1 / \partial \alpha$ in the iterative process (6)–(7) not only for the spectral region of photosynthetically active radiation but for the near-infrared region as well.

CALCULATION OF THE BIDIRECTIONAL REFLECTANCE FACTOR

This section is a brief summary of the paper of Antyufeev and Marshak (1990). We consider a flat, horizontal leaf canopy of the leaf area index H, which is illuminated from above by diffuse and direct radiation, i.e.,

$$I(0, \mathbf{\Omega}) = I_0 \delta(\mathbf{\Omega} - \mathbf{\Omega}_0) + I_d(\mathbf{\Omega}).$$

At the ground surface, it is assumed that a fraction r_s of the energy reaching the ground through the canopy is reradiated isotropically back into the canopy,

$$I(H, \mathbf{\Omega}) = \frac{r_s}{\pi} \int_{\{2\pi^-\}} |\mu'| I(H, \mathbf{\Omega}') \, d\mathbf{\Omega}'.$$

Here, I is the radiance distribution function, I_0 is the intensity of the monodirectional solar radiation in the direction $\mathbf{\Omega}_0$, I_d is the diffuse solar radiance, and function δ is the Dirac delta function.

We denote the product $I(t,\mathbf{\Omega})G(\mathbf{\Omega})$ by $J(t,\mathbf{\Omega})$. One can write then the integral transport equation as follows:

$$J(t,\mathbf{\Omega}) = \int_{\{4\pi\}}\int_0^H k[(t',\mathbf{\Omega}') \to (t,\mathbf{\Omega})] \times J(t',\mathbf{\Omega}')\, dt'\, d\Omega' + Q(t,\mathbf{\Omega}), \quad (8)$$

where

$$Q(t,\mathbf{\Omega}) = I(0,\mathbf{\Omega})G(\mathbf{\Omega}) \times \exp[-G(\mathbf{\Omega})t/|\mu|], \quad \mu < 0. \quad (9)$$

The kernel $k(x' \to x)$, where $x \sim (t,\mathbf{\Omega})$ is a point in the phase space X, is expressed by (Antyufeev and Marshak, 1990)

$$k[(t',\mathbf{\Omega}') \to (t,\mathbf{\Omega})] = \begin{cases} P(\mathbf{\Omega}' \to \mathbf{\Omega})\dfrac{G(\mathbf{\Omega})}{|\mu|}\exp\left[-\displaystyle\int_{t'}^{t}\frac{\sigma_\kappa(\tau,\mathbf{\Omega}',\mathbf{\Omega})}{|\mu|}d\tau\right], & (t-t')\mu < 0, \\ 0, & (t-t')\mu > 0. \end{cases} \quad (10)$$

Solving the transport equation (8), the BDRF in the direction $\mathbf{\Omega}^*$ can be found as

$$R(\mathbf{\Omega}^*) = \pi J(0,\mathbf{\Omega}^*)/[G(\mathbf{\Omega}^*)A], \quad (11)$$

where

$$A = I_0|\mu_0| + \int_{\{2\pi^-\}} |\mu'| I_d(\mathbf{\Omega}')\, d\mathbf{\Omega}'.$$

Equation (8) is solved by the Monte Carlo method (Mikhailov, 1974; Antyufeev and Marshak, 1990). We rewrite it in operator notation as

$$J = KJ + Q, \quad (12)$$

where K is the integral operator with the kernel $k(x' \to x)$ defined by (10). It is known that if $\|K\| < 1$, the unique solution of (12) can be written as (Kantorovich and Akilov, 1978)

$$J = Q + KQ + K^2Q + \cdots.$$

Let the scalar product in the phase space X be

$$(\psi,\varphi) = \int_X \psi(x)\varphi(x)\, dx = \int_0^H\int_{\{4\pi\}} \psi(t,\mathbf{\Omega})\varphi(t,\mathbf{\Omega})\, d\mathbf{\Omega}\, dt.$$

Then,

$$\begin{aligned} J(0,\mathbf{\Omega}^*) = J(x^*) &= (J,\delta_{x^*}) \\ &= (Q,\delta_{x^*}) + (KQ,\delta_{x^*}) + (K^2Q,\delta_{x^*}) + \ldots \\ &= (Q,K^*\delta_{x^*}) + (KQ,K^*\delta_{x^*}) \\ &\quad + (K^2Q,K^*\delta_{x^*}) + \cdots. \end{aligned} \quad (13)$$

Here, $x^* \sim (0,\mathbf{\Omega}^*)$, and δ_{x^*} is the Dirac delta function;

$$\int_X \varphi(x)\,\delta_{x^*}(x)\, dx = \varphi(x^*),$$

the operator K^* is the operator adjoint to K, and

$$[K^*\delta_{x^*}](x) = \Psi(x)G(\mathbf{\Omega}^*),$$

where the contribution function $\Psi(x)$ is

$$\Psi(x) = \Psi(t,\mathbf{\Omega}) = P(\mathbf{\Omega} \to \mathbf{\Omega}^*)\frac{1}{\mu^*} \times \exp\left[-\int_0^t \frac{\sigma_\kappa(t',\mathbf{\Omega},\mathbf{\Omega}^*)}{\mu^*}dt'\right], \quad \mu^* > 0. \quad (14)$$

It follows from (9), (11), (13), and (14) that

$$R(\mathbf{\Omega}^*) = (\bar{Q},\Psi) + (K\bar{Q},\Psi) + (K^2\bar{Q},\Psi) + \cdots, \quad (15)$$

where

$$\bar{Q}(t,\mathbf{\Omega}) = Q(t,\mathbf{\Omega})\pi/A. \quad (16)$$

So, the ith term on the right-hand-side of (15) is the contribution of ith-order scattered photons to the estimation of the BDRF. Expansion (15) corresponds to the following algorithm of the Monte Carlo method; namely, according to the transfer kernel $k(x' \to x)$, the random Markov chain $x_0^n \to x_1^n \to x_2^n \to \cdots \to x_m^n$ is simulated, where m is the random number of the last interaction. After each interaction at the point x_i^n the contribution $[W_i^n\Psi(x_i^n)]$ is included in the statistical estimation R and

$$R(\mathbf{\Omega}^*) \approx \frac{1}{N}\sum_{n=1}^{N}\sum_{i=0}^{m} W_i^n\Psi(x_i^n), \quad (17)$$

where N is the total number of trajectories, W_i^n is the "weight" of the nth photon after the ith interaction. In case of reflection from the soil, the contribution function $\Psi = \Psi_s$, where

$$\Psi_s(t,\mathbf{\Omega}) = \frac{r_s}{\pi}\frac{|\mu|}{G(\mathbf{\Omega})} \times \exp\left[-\int_0^t \frac{\sigma_\kappa(t',\mathbf{\Omega},\mathbf{\Omega}^*)}{\mu^*}\,dt'\right]\delta(t-H), \quad \mu^* > 0. \quad (18)$$

Here, r_s is the soil albedo and $|\mu|/\pi$ is the angle density of reflection from the "Lambertian" soil surface.

CALCULATION OF THE DERIVATIVES

Let us rewrite the Neuman's series (15) in the following form

$$R = \int Q_0\Psi_0 + \int Q_0k_{01}\Psi_1 + \int Q_0k_{01}k_{12}\Psi_2 + \cdots. \quad (19)$$

We have written $\int Q_0k_{01}\Psi_1$ instead of

$$(K\overline{Q},\Psi) = \int_X (K\overline{Q})(x_1)\Psi(x_1)\,dx_1 = \int_X\left[\int_X k(x_0\to x_1)\overline{Q}(x_0)\,dx_0\right]\Psi(x_1)\,dx_1 = \int_X\int_X \overline{Q}(x_0)k(x_0\to x_1)\Psi(x_1)\,dx_0\,dx_1,$$

and so on. For the calculation of $\partial R/\partial\alpha$ we differentiate the series (19). Let

$$f' = \partial f/\partial\alpha,$$

then

$$R' = \int [Q_0'\Psi_0 + Q_0\Psi_0'] + \int [Q_0'k_{01}\Psi_1 + Q_0k_{01}'\Psi_1 + Q_0k_{01}\Psi_1'] + \cdots = \int Q_0\Psi_0\left[\frac{Q_0'}{Q_0} + \frac{\Psi_0'}{\Psi_0}\right] + \int Q_0k_{01}\Psi_1 \times\left[\frac{Q_0'}{Q_0} + \frac{k_{01}'}{k_{01}} + \frac{\Psi_1'}{\Psi_1}\right] + \cdots = \int Q_0\Psi_0W_0 + \int Q_0k_{01}\Psi_0W_{01} + \cdots. \quad (20)$$

The last expression corresponds to the following scheme of calculation: as before, we simulate the Markov chain of interactions, $x_0^n \to x_1^n \to x_2^n \to \cdots \to x_m^n$, but unlike the BDRF estimation (17), the contribution $[\Psi(x_i^n)W_{0\cdots i}]$ is included instead $[\Psi(x_i^n)]$ in the statistical estimation $\partial R/\partial\alpha$ at the point of interaction x_i^n. So, the derivatives $\partial R/\partial\alpha$ are calculated along the same trajectories as the BDRF. Such a modification allows us to economize on the computer time. Strict grounds of the statistical estimation (20) can be found in Mikhailov (1974). The labor-intensiveness of the calculation of derivatives, in comparison to the BDRF calculation, is defined by the labor-intensiveness of the calculation of the "weight" $W_{0\cdots i}$.

As we have already noted, the calculation of $W_{0\cdots i}$ with sufficient accuracy demands significant computer time. This is why we simplify the problem by calculating the derivatives of the first term in expansion (15). Let $R_1 = \int Q_0\Psi_0$, then for the estimation $\partial R_1/\partial\alpha$, it is sufficient to calculate the "weight"

$$W_0 = Q_0'/Q_0 + \Psi_0'/\Psi_0$$

only.

Let us write the expression for R_1. There are two types of interactions: at a leaf surface and at the soil surface. Then,

$$R_1 = R_{1L} + R_{1S}, \quad (21)$$

where R_{1L} is the contribution to the BDRF of photons scattered from the leaves and R_{1S} is the contribution of photons reflected from the soil. From (14)–(16) we have

$$R_{1L} = \frac{\pi}{A}\frac{I_0G(\mathbf{\Omega}_0)P(\mathbf{\Omega}_0\to\mathbf{\Omega}^*)}{\mu^*} \times\int_0^H \exp\left[-\frac{G(\mathbf{\Omega}_0)t}{|\mu_0|} - \int_0^t\frac{\sigma_\kappa(t',\mathbf{\Omega}_0,\mathbf{\Omega}^*)}{\mu^*}\,dt'\right]dt + \frac{\pi}{A}\int_{\{2\pi^-\}}\frac{I_d(\mathbf{\Omega}')G(\mathbf{\Omega}')P(\mathbf{\Omega}'\to\mathbf{\Omega}^*)}{\mu^*} \times\int_0^H \exp\left[-\frac{G(\mathbf{\Omega}')t}{|\mu'|} - \int_0^t\frac{\sigma_\kappa(t',\mathbf{\Omega}',\mathbf{\Omega}^*)}{\mu^*}\,dt'\right] \times dt\,d\mathbf{\Omega}', \quad (22)$$

and from (15), (16), and (18) it follows that

$$R_{1S} \doteq \frac{r_s}{A} I_0|\mu_0| \times \exp\left[-\frac{G(\boldsymbol{\Omega}_0)H}{|\mu_0|} - \int_0^H \frac{\sigma_\kappa(t',\boldsymbol{\Omega}_0,\boldsymbol{\Omega}^*)}{\mu^*}\,dt'\right] + \frac{r_s}{A}\int_{\{2\pi^-\}} |\mu'| I_d(\boldsymbol{\Omega}')\exp\left[-\frac{G(\boldsymbol{\Omega}')H}{|\mu'|} - \int_0^H \frac{\sigma_\kappa(t',\boldsymbol{\Omega}',\boldsymbol{\Omega}^*)}{\mu^*}\,dt'\right] d\Omega'. \quad (23)$$

Now, we consider the statistical estimations $\partial R_1/\partial\alpha$ with respect of concrete parameters α.

1. *The albedo of soil surface r_s*. It is clear that only R_{1S} depends on r_s. Then $W_0 = 1/r_s$ and

$$\frac{\partial R_1}{\partial \alpha} = A^{-1} I_0|\mu_0| \times \exp\left[-\frac{G(\boldsymbol{\Omega}_0)H}{|\mu_0|} - \int_0^H \frac{\sigma_\kappa(t',\boldsymbol{\Omega}_0,\boldsymbol{\Omega}^*)}{\mu^*}\,dt'\right] + A^{-1}\int_{\{2\pi^-\}} |\mu'| I_d(\boldsymbol{\Omega}')\exp\left[-\frac{G(\boldsymbol{\Omega}')H}{|\mu'|} - \int_0^H \frac{\sigma_\kappa(t',\boldsymbol{\Omega}',\boldsymbol{\Omega}^*)}{\mu^*}\,dt'\right] d\boldsymbol{\Omega}'.$$

2. *Coefficients of reflectance r_L and transmittance t_L*. Only the leaf phase function f depends on these parameters. Let $\alpha = r_L$ or $\alpha = t_L$, then

$$W_0 = \frac{\Psi'_\alpha}{\Psi} = \frac{P'_\alpha(\boldsymbol{\Omega}\to\boldsymbol{\Omega}^*)}{P(\boldsymbol{\Omega}\to\boldsymbol{\Omega}^*)} = \frac{f'_\alpha(\boldsymbol{\Omega}_L;\boldsymbol{\Omega}\to\boldsymbol{\Omega}^*)}{f(\boldsymbol{\Omega}_L;\boldsymbol{\Omega}\to\boldsymbol{\Omega}^*)},$$

where functions P and f are defined by (3) and (4), respectively. Substituting in the last equality $\alpha = r_L$, we get

$$W_0 = W_{0r_L} = \begin{cases} |\boldsymbol{\Omega}^*\cdot\boldsymbol{\Omega}_L|/\pi, \\ (\boldsymbol{\Omega}^*\cdot\boldsymbol{\Omega}_L)(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}_L) < 0, \\ 0, \\ (\boldsymbol{\Omega}^*\cdot\boldsymbol{\Omega}_L)(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}_L) > 0, \end{cases}$$

and correspondently if $\alpha = t_L$, then

$$W_0 = W_{0t_L} = \begin{cases} 0, \\ (\boldsymbol{\Omega}^*\cdot\boldsymbol{\Omega}_L)(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}_L) < 0, \\ |\boldsymbol{\Omega}^*\cdot\boldsymbol{\Omega}_L|/\pi, \\ (\boldsymbol{\Omega}^*\cdot\boldsymbol{\Omega}_L)(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}_L) > 0. \end{cases}$$

3. *Parameters b and c characterizing the density of leaf angle distribution*. There are two functions Ψ and $\overline{Q}$ [definitions (14) and (16), respectively] that depend on these parameters, namely,

$$\frac{\overline{Q}_\alpha}{\overline{Q}} = \frac{G'_\alpha}{G} - \frac{t}{\mu}G'_\alpha,$$

$$\frac{\Psi'_\alpha}{\Psi} = \frac{P'_\alpha(\boldsymbol{\Omega}\to\boldsymbol{\Omega}^*)}{P(\boldsymbol{\Omega}\to\boldsymbol{\Omega}^*)} - \int_0^t \left[\frac{\sigma_\kappa(t',\boldsymbol{\Omega},\boldsymbol{\Omega}^*)}{\mu^*}\right]'_\alpha dt'. \quad (24)$$

Thus,

$$W_{0\alpha} = \frac{\overline{Q}'_\alpha}{\overline{Q}} + \frac{\Psi'_\alpha}{\Psi}.$$

Considering separately the cases $\alpha = b$ and $\alpha = c$, we find the values of the derivatives. We note that the integral in the second term on the right-hand part of (24) can be evaluated analytically.

4. *Parameter H (LAI)*. It follows from (21)–(23) that the parameter H is included in the expressions (22)–(23) and in the definition (2). We assume here for simplification that $I_d \equiv 0$. Then differentiating R_{1L} with respect to H, we get

$$\frac{\partial R_{1L}}{\partial H} = \frac{\pi G(\boldsymbol{\Omega}_0)P(\boldsymbol{\Omega}_0\to\boldsymbol{\Omega}^*)}{|\mu_0|\mu^*} \times \exp\left[-\frac{G(\boldsymbol{\Omega}_0)H}{|\mu_0|} - \int_0^H \frac{\sigma_\kappa(t',\boldsymbol{\Omega}_0,\boldsymbol{\Omega}^*)}{\mu^*}\,dt'\right] - \frac{\pi G(\boldsymbol{\Omega}_0)P(\boldsymbol{\Omega}_0\to\boldsymbol{\Omega}^*)}{|\mu_0|\mu^*} \times \int_0^H \exp\left[-\frac{G(\boldsymbol{\Omega}_0)t}{|\mu_0|} - \int_0^t \frac{\sigma_\kappa(t',\boldsymbol{\Omega}_0,\boldsymbol{\Omega}^*)}{\mu^*}\,dt'\right] \times \frac{\partial}{\partial H}\left[-\int_0^t \frac{\sigma_\kappa(t',\boldsymbol{\Omega}_0,\boldsymbol{\Omega}^*)}{\mu^*}\,dt'\right] dt.$$

So, the derivative of R_{1L} with respect to H is equal to the sum of two components: The first one is the analytical expression and the second one is the mathematical expectation of the statistical estimation of R_{1L} with the weight

$$W = \int_0^t \frac{\partial}{\partial H}\left[\frac{\sigma_\kappa(t',\boldsymbol{\Omega}_0,\boldsymbol{\Omega}^*)}{\mu^*}\right] dt'.$$

By analogy, we have

$$\frac{\partial R_{1S}}{\partial H} = -R_{1S}\left\{\frac{G(\boldsymbol{\Omega}_0)}{|\mu_0|} + \frac{\sigma_\kappa(H,\boldsymbol{\Omega}_0,\boldsymbol{\Omega}^*)}{\mu^*} + \int_0^H \frac{\partial}{\partial H}\left[\frac{\sigma_\kappa(t',\boldsymbol{\Omega}_0,\boldsymbol{\Omega}^*)}{\mu^*}\right] dt'\right\}$$

and

$$\frac{\partial R_1}{\partial H} = \frac{\partial R_{1L}}{\partial H} + \frac{\partial R_{1S}}{\partial H}.$$

It is not difficult to repeat the above calculations taking also into account the diffuse component.

5. *Parameter κ, characterizing leaves dimensions*. The contribution functions (14) and (18) depend on σ_κ. Then,

$$W_{0\kappa} = \frac{\Psi'_\kappa}{\Psi} = \frac{\Psi'_{s\kappa}}{\Psi_s} = -\int_0^t \frac{\partial}{\partial \kappa}\left[\frac{\sigma_\kappa(t', \mathbf{\Omega}, \mathbf{\Omega}^*)}{\mu^*}\right] dt'.$$

NUMERICAL RESULTS

We shall now discuss here some results of model calculations for estimating canopy parameters from the BDRF or from the transmittance function (depending on the parameter desired). The general scheme in the simplest case is the following: one of the parameters (or a couple of homogeneous parameters as r_L and t_L or b and c) are considered as unknown and are estimated by the algorithm proposed above. Other parameters are kept fixed. The iteration is stopped if the first two significant numbers of the estimate coincide with the exact solution. We consider two schemes. The first one (standard scheme) requires to calculate the full derivatives $\partial R / \partial \alpha$ in the iterative process (6)–(7). The second one (modified scheme) uses only the derivatives of the first-order scattering photons: $\partial R_1 / \partial \alpha$.

In Table 1, results of inversion are given for a "thick" canopy ($H = 4$) in the near-infrared spectral region ($r_L = t_L = 0.46$, $r_s = 0.2$) where the role of multiply-scattered photons is quite significant in comparison to the photosynthetically active region. The diffuse incident radiation is absent.

Table 1. Some Numerical Results for Estimating Three Optical Canopy Parameters (Coefficient of Leaf Reflectance r_L, Coefficient of Leaf Transmittance t_L, and Soil Albedo r_s) and Four Geometrical Canopy Parameters (Leaf Area Index H, Leaf Size Parameter κ, and Two Parameters of Leaf Angle Distribution: b and c)

	Canopy Parameters						
Row	r_L	t_L	r_s	H	κ	b	c
1. Exact values of parameters	0.46	0.46	0.2	4.0	0.08	1	1
2. The initial guess	0.20	0.20	0.1	2.0	0.04	0	0
3. Number of iterations for the standard scheme	3	3	2	2	—	—	—
4. Number of iterations for the modified scheme	3	3	5	5	2	5	5
5. Errors (%)	1	2	2	2	1	20	30

The first row of Table 1 corresponds to the "desired" parameters; the second row describes the first-order approximation to the solution or the initial guess. The number of iterations required to obtain given accuracy for the standard scheme are presented in the third row, and the fourth row illustrates the number of iterations needed for the modified scheme. The parameter κ, characterizing the size of leaves, was estimated quickly by the modified scheme; thus, it was not estimated by the standard method. However, the parameters of leaf angle distribution (b and c) could not be successfully estimated by the standard scheme (Table 1, blank entry on row 3, columns 7 and 8). It is quite clear that the number of iterations for the modified method cannot be less than for the standard one (rows 3 and 4) since the theoretical rate of convergence of the iterative process becomes slower. However, for some parameters (b and c) it was fully compensated by the more accurate calculations of the derivatives $\partial R_1 / \partial b$ and $\partial R_1 / \partial c$. Similar calculations for a "thin" canopy ($H = 2$) allowed us to estimate parameters b and c to within 10% after five iterations. It shows that, as is expected, the problem is more easily solved for canopies with less leaf area index.

CONCLUSIONS

In the present paper we have continued the development of the canopy reflectance model proposed by Antyufeev and Marshak (1990). We described the technique for estimating canopy parameters and showed that the Monte Carlo model for solving the transport equation in leaf canopies is invertible.

Two different schemes for calculation of the derivatives of the BDRF with respect to the unknown parameters were considered. Both of them calculate derivatives by Monte Carlo technique, using the same photon trajectories as for calculating the BDRF. The modified scheme that used the derivatives of the first-order scattering photons was more effective and allowed us to estimate the parameters of leaf angle distribution (especially for not large LAI). Preliminary results presented here give us hope that the parameters of a more complicated model described by the integral equation of radiative transfer, [for instance, the model proposed in the recent paper of Myneni, Marshak, and Knyazikhin (1990)], can be estimated as well. However, a more effective modification of proposed scheme should be developed.

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