MODELLING CANOPY REFLECTANCE WITH SPECTRAL INVARIANTS

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ABSTRACT:

The concept of using spectral invariants to describe the scattering and absorption processes in a vegetation canopy has been developed for application to remote sensing studies in recent years. It has been shown that an average 'recollision probability' can describe the main impacts of structure on directional-hemispherical scattering and transmission, and there has been some indication that this might provide a useful route to modelling canopy reflectance. In this paper, we examine how an existing formulation of canopy reflectance and transmittance describes radiometric behaviour as a function of scattering order. We note that the assumptions underlying the model break down for moderate to high leaf area index (LAI), and show that this leads to a poor description of scattering as a function of interaction order. This leads to the model parameters losing any direct biophysical meaning, becoming 'effective' terms. It is shown that it is useful to maintain the direct meaning of the parameters, as this potentially simplifies the modelling of bi-directional fluxes and the dependence of parameters on zenith angle and leaf scattering asymmetry. We propose a new formulation that maintains the small number of parameters in the original model but better describes the scattering behaviour.

1. INTRODUCTION

1.1 Canopy spectral invariants

The total scattering from a vegetation canopy at optical wavelengths, S_{λ} , can be expressed as a function of wavelength λ by:

$$S_{\lambda} = t_0 + \left(1 - t_0\right) \sum_{i=1}^{1 - \infty} s_i \omega_{\lambda}^i \tag{1}$$

where t_0 is the probability of radiation being transmitted through the canopy without interacting with canopy elements (the zeroorder transmittance), ω is the canopy element single scattering albedo and the terms s_i are spectrally-invariant terms dependent on the incident radiation distribution, the arrangement and angular distribution of canopy elements, and the ratio ζ_{λ} of leaf

reflectance $R_{leaf,\lambda}$ to total leaf scattering $(\omega_{\lambda} = R_{leaf,\lambda} + T_{leaf,\lambda})$:

$$\zeta_{\lambda} = R_{leaf,\lambda} / \left(R_{leaf,\lambda} + T_{leaf,\lambda} \right)$$
⁽²⁾

The canopy spectral transmittance $T_{bs,\lambda}$ and reflectance $R_{bs,\lambda}$ for a canopy with a totally absorbing lower boundary ('black soil') can be expressed in similar forms to (1):

$$T_{bs,\lambda} = t_0 + (1 - t_0) \sum_{i=1}^{1-\infty} t_{bs,i} \omega_{\lambda}^i$$
(3a)

$$R_{bs,\lambda} = (1 - t_0) \sum_{i=1}^{1 - \infty} r_{bs,i} \omega_{\lambda}^{i}$$
(3b)

where $t_{bs,i}$, $r_{bs,i}$ are spectrally-invariant terms expressing the proportion of radiation scattered through the lower and upper canopy boundaries relative to the radiation initially intercepted by canopy foliage. Absorptance is found from energy conservation.

This is a convenient statement of canopy reflectance and transmittance because it separates the 'geometric' aspects of scattering (the spectral invariants) from those dependent on wavelength (leaf single scattering albedo). We can express $T_{total,\lambda}$, $R_{total,\lambda}$, the transmittance and reflectance of a canopy with an underlying Lambertian lower boundary of reflectance $R_{s,\lambda}$ following Knyazikhin and Marshak (2000) and Wang et al. (2003), but in this paper, we only consider the black soil 'component' of the canopy.

Various authors, summarised by Huang et al. (2007), have built models of canopy radiation interactions through assumptions regarding photon recollision and escape probabilities in a canopy. The recollision probability at scattering order *i*, p_i is the probability that photons that have interacted with canopy elements at scattering order *i*-1 will recollide with canopy elements. The escape probability can be partitioned into the upward escape probability, ρ_i and the downward probability, τ_i . Then:

$$p_i + \rho_i + \tau_i = 1 \tag{4}$$

from consideration of energy conservation. The spectrallyinvariant terms in equation (3) can be expressed using recollision and escape probabilities:

$$r_i = \rho_i \prod_{j=1}^{j=i-1} p_j \tag{5a}$$

$$t_i = \tau_i \prod_{j=1}^{j=i-1} p_j \tag{5b}$$

The total scattering spectral invariants s_i in equation (1) are:

$$s_i = t_i + r_i \tag{5c}$$

Under conditions of zero absorptance ($\omega = 1$), the radiance on the leaves at interaction order *i* must be entirely scattered out of the canopy over all orders greater than *i*. Thus:

$$\sum_{j=i+1}^{j=\infty} s_j = s_i \tag{5d}$$

where s_0 is defined as unity.

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1.2 Monte Carlo simulations

We performed simulations of canopy directional-hemispherical reflectance and transmittance using a reverse Monte Carlo Ray Tracer (MCRT) drat (Lewis, 1999, modified as described in Saich et al., 2001; Disney et al., 2006), for a range of zenith angles. We did further simulations of bidirectional reflectance and transmittance, although they are not analysed in this paper. The MCRT tool drat can output results as a function of scattering order, from which we can directly simulate r_i and t_i . This allows the reflectance and transmittance to be calculated for arbitrary leaf albedo. Ray interactions are followed up to scattering order 100 in the simulations and an analytical approximation applied for further interactions (Appendix 1).

We simulated a range of canopy structures. Here we present results for homogeneous (LAI 1-20) and spherically-clumped canopies (LAI 5). The homogeneous canopies are composed of explicit representations of non-overlapping disks with a uniform angular distribution and radius 0.02 units and canopy vertical extent 5 x LAI. ζ varies between 0.2 and 0.6 for these simulations. The spherically-clumped canopy is that of RAMI scene HET01¹. It has disc leaves with a radius of 0.1 units contained in spheres of 15 unit radius distributed over a 100 unit x 100 unit area (infinitely repeated in horizontal extent) (see¹ for further details)

1.3 Some initial observations on recollision and escape probabilities

Figure 1 shows recollision probabilities for homogeneous canopies as a function of scattering order at varying values of LAI with equal leaf reflectance and transmittance, for directional-hemispherical fluxes at a zenith angle of 0° .

The recollision probability tends to converge to a final value after relatively few iterations, at least for low to moderate LAI. Lewis and Disney (2007) note that the number of iterations until convergence is approximately equal to the LAI. This final value, p_{∞} , can be considered the recollision probability of the radiation in the canopy when it is 'well mixed' (i.e. the radiation distribution in the canopy has settled down to some final function and does not change much with each iteration). Alternatively, Panferov et al. (2001) note this as the principal eigenvalue of the radiative transfer operator.

Figure 2 shows the escape probabilities corresponding to the recollision probabilities in Figure 1. These again converge to some 'well-mixed' values, ρ_{∞} and τ_{∞} in the upward and downward directions respectively, but convergence does not occur until around 2 x LAI interactions. Further, there is an approximate symmetry (in log space) between the two escape probabilities. At and after the point of convergence, the probabilities become equal, so from (4):

$$\rho_{\infty} = \tau_{\infty} = \frac{1}{2} \left(1 - p_{\infty} \right) \tag{6}$$



Figure 1. Recollision probability as a function of scattering order for LAI 1, 5 and 10, $\zeta = 0.5$, zenith 0°.



Figure 2. Upward and downward escape probabilities as a function of scattering order for homogeneous canopies at LAI 1, 5 and 10, $\zeta = 0.5$, zenith angle 0°.

1.4 Previous models using spectral invariants

Previous models assume that the recollision probability p_i is constant with scattering order (Huang et al., 2007). We denote this constant value p_{eff} . Under this assumption and with the energy conservation constraint (5d), we can write the total scattering through:

$$S_{R,\lambda} = \frac{S_{R,\lambda} - t_0}{1 - t_0} = \frac{(1 - p_{eff})\omega_{\lambda}}{1 - p_{eff}\omega_{\lambda}}$$
(7a)

where $S_{R,\lambda}$ is the relative total scattering. The effective recollison probability p_{eff} is less than p_{∞} . Canopy relative transmittance $T_{R,\lambda}$ can be stated as:

$$T_{R,\lambda} = \frac{T_{\lambda,\theta} - t_{0,\theta}}{\left(1 - t_{0,\theta}\right)} = \frac{t_{0,equiv}}{\left(1 - t_{0,equiv}\right)} \frac{p_{t}\omega_{\lambda}}{\left(1 - p_{t}\omega_{\lambda}\right)}$$
(7b)

(Shabanov et al., 2003; Huang et al., 2007) where $t_{0.equiv}$ is an effective value for zero-order transmittance. p_t is understood to be an equivalent recollision probability for radiation escaping through the canopy lower boundary. Shabanov et al. (2003) define p_t as the eigenvalue normalised by leaf albedo of the linear operator that assigns downward radiances at the canopy bottom to incoming radiation, but other than that it has no direct physical meaning. We see $t_{0,0}p_t/(1-t_{0,0})$ as the assumed model for escape probability in the downward direction, τ_t , so:

¹http://rami-benchmark.jrc.it/HTML/RAMI3/EXPERIMENTS3/ HETEROGENEOUS/FLOATING_SPHERES/ SOLAR_DOMAIN/DISCRETE/DISCRETE.php

$$T_{R,\lambda} = \frac{\tau_{I}\omega_{\lambda}}{\left(1 - p_{I}\omega_{\lambda}\right)}$$
(7c)

From equations (7a) and (7c) and consideration of energy conservation, we can infer the relative reflectance $R_{R,\lambda}$ to be:

$$R_{R,\lambda} = S_{R,\lambda} - T_{R,\lambda} = \frac{(1 - p_{equiv})\omega_{\lambda}}{(1 - p_{equiv}\omega_{\lambda})} - \frac{\tau_{\iota}\omega_{\lambda}}{(1 - p_{\iota}\omega_{\lambda})}$$
(7d)

Equations (7a,c,d) describe canopy directional-hemispherical reflectance and transmittance. They have only five parameters $(t_{0,\theta}, p_{equiv}, \tau_t, p_t, \omega_{\lambda})$ —four of these are independent of wavelength. The spectral invariants p_{equiv}, τ_t, p_t can be inferred from measurements of $T_{\lambda,\theta}$ and $R_{\lambda,\theta}$, given additional measurements of direct transmittance $t_{0,\theta}$ (gap probability) and leaf single scattering albedo ω_{λ} . Alternatively, $t_{0,\theta}$ can be calculated from analytical or numerical radiative transfer models and p_{equiv}, τ_t and p_t inferred from simulations of the behaviour of $T_{\lambda,\theta}$ and $R_{\lambda,\theta}$ as a function of ω_{λ} .



Figure 3a. Relative reflectance, transmittance and total scattering as a function of leaf single scattering albedo, for the canopies (A,B,C,D) for ζ=0.5, zenith 0° (symbols), with lines showing fitting of the original model.



Figure 3b. Root mean square error (RMSE) for relative reflectance, transmittance and total scattering for the homogeneous canopies as a function of LAI.

Figure 3 shows the results of fitting the model presented above (the 'original model') to MCRT simulations of the relative reflectance, transmittance and total scattering for four canopies. Canopies A, B and C are homogeneous with LAI 1, 5 and 10 respectively. Canopy D is the RAMI heterogeneous canopy. The model fits the 'observed' (i.e. MCRT results) well in both cases (Figure 3b). Figure 3c shows that, except for very low LAI, the form of spectrally-invariant terms as a function of interaction order implied by the original model is inappropriate. Indeed, for moderate or high LAI (Figure 3cB,C) the assumed form for both reflectance and transmittance depart dramatically from the observed behaviour.

One could argue that this is unimportant: the models fit the observations and the departures noted are for relatively high scattering orders where the contributions are low. But the contribution of high order scattering terms is proportional to $[\omega p_{\infty}]^{l}$, so for example, $\omega p_{\infty}=0.99$, contributions of photons scattered 100 times are still as high as $[0.99]^{100}=37\%$. Clearly for low ωp_{∞} the model is works well, but using inappropriate functions means that all model parameters lose any physical meaning (they all become effective terms) and any interpretation of first order scattering terms, bidirectional terms or parameter behaviour with varying ζ or zenith angle lose clarity as well.



Figure 3c. Spectrally-invariant terms as a function of scattering order for canopies A, B, C and D for ξ =0.5, zenith 0° (symbols), with lines showing the original model.

For these reasons, we seek in this paper to establish an improved set of descriptors based around the concepts of spectral invariance. This will be achieved by more careful consideration of the modelling of escape probabilities. The next section examines scattering behaviour as a function of ζ and zenith angle.

2. FURTHER INVESTIGATION OF SCATTERING AS A FUNCTION OF INTERACTION ORDER

2.1 Behaviour as a function of ζ



Figure 4. (a-d) Escape probabilities for varying ξ , LAI=5, zenith angle 0°.

Figure 4 shows the variation in escape probability with $\boldsymbol{\zeta}$ for the canopy with LAI 5. We note that the interaction order of convergence appears to remain constant and that the initial escape probabilities ρ_1, τ_1 decrease with increasing $\boldsymbol{\zeta}$. If we represent the first order escape probabilities $\tau_{1\boldsymbol{\zeta}}$ and $\rho_{1\boldsymbol{\zeta}}$ by:

$$\tau_{1\xi} = A_1 (1 - \zeta) + A_3 \zeta \tag{8a}$$

$$\rho_{1\zeta} = \left(A_2 (1 - \zeta) + A_4 \zeta \right) / (1 - t_{0,\vartheta})$$
(8b)

then:

$$\tau_{1\zeta} = A_1 + \frac{\zeta}{0.5} \left(\tau_{1\zeta=0.5} - A_1 \right)$$
(8c)

$$\rho_{1\xi} = A_2 + \frac{\xi}{0.5} \left(\rho_{1\xi=0.5} - A_2 \right)$$
(8d)

Escape (and therefore recollision) probabilities show a much weaker dependence on ζ for $i \ge 2$.



Figure 5. (a) ρ_{∞} as a function of LAI for varying $\boldsymbol{\zeta}$; (b) p_{∞} for varying values of $\boldsymbol{\zeta}$ as a function of $p_{\infty}(\boldsymbol{\zeta} = 0.5)$.

Figure 5a shows the variation in infinite scattering order escape probability ρ_{∞} with LAI and ξ . The variation with ξ is relatively small compared to that with LAI or the variation in first order escape probabilities, but shows a linear dependency. This is further emphasised in Figure 5b where we see that:

$$p_{\infty}(\zeta) = p_{\infty}(\zeta = 0.5) - A_5 p_{\infty}(\zeta - 0.5)$$
(8e)

Here, A_5 is calibrated to be 0.22.

2.2 Behaviour as a function of zenith angle



Figure 6. Escape probabilities for varying zenith, LAI=5, ξ =0.5.

Figure 6 shows escape probabilities for LAI 5 for varying zenith angles. ρ_{∞} appears to be invariant with zenith angle (this is not quite true for ρ_{equiv} which varies with zenith angles greater than around 60° (Smolander and Stenberg, 2005)). There is generally small variation in the initial escape probabilities with zenith angle, although a small increase is seen at high angles (zenith greater than 60°).

3. BUILDING A NEW MODEL

3.1 A model based on escape probabilities

Given the observations above, we propose a model relating escape probabilities:

$$\sqrt{\tau_i \rho_i} = a_1 \tag{9a}$$

$$\sqrt{\frac{\tau_i}{\rho_i}} = \sqrt{\frac{r_i}{t_i}} = 1 - a_2^{i+1}$$
(9b)

Equation (9a) arises from the observation of near symmetry in log space of the escape probabilities. Equation (9b) is an empirical model that describes the square root of the escape ratios as shown in Figure 7.



Figure 7. MCRT simulations of the square root of the ratio of downward to upward escape probabilities for canopies A, B, C and D.

From equation (9), we can formulate for the escape probabilities:

$$\rho_i = \frac{a_1}{\left(1 - a_2^{i+1}\right)}$$
(10a)

$$r_i = a_1 \left(1 - a_2^{i+1} \right) \tag{10b}$$

The recollision probability is found from equation (4). This fully specifies the reflectance model by calculating the terms r_i and t_i from equation (5) and the black soil reflectance and transmittance through equation (3). The model effectively has 3 parameters, a_2 , t_0 and p_{∞} —since a_1 can be eliminated through energy conservation.



Figure 8. RMSE in model fit for the new model as a function of LAI for ζ 0.5, zenith angle 0°.



Figure 9. Spectrally-invariant terms as a function of scattering order for canopies A, B, C and D for ζ =0.5, zenith 0° (symbols), with lines showing fitting of the new model

Figure 8 shows the RMSE in model fit as a function of LAI for the homogeneous canopies. Clearly this fits the MCRT simulation much better than the original model, with RMSE being mostly less than 0.05. Figure 9 shows the reflectance and transmittance terms reconstructed by fitting this model to data for canopies A, B, C and D. Comparing this with Figure 3 we can see that the fidelity of the spectral invariants is much greater. We can recognise in particular that p_{∞} mostly maintains its original meaning (it still tends to be very slightly underestimated). We can consider this a successful model, in that the considerations of varying ζ , zenith angle etc. considered above can be easily incorporated into the model. The single main drawback is that the spectral invariants have to be calculated as products and sums of infinite series. In practice, we can resort to simpler analytical formulations for scattering orders greater than around twice the LAI, but the fact that the model cannot be simply stated in analytical form may limit its application.

3.2 A simpler analytical model

With this in mind, we develop a simpler analytical model that will achieve much the same ends as the new model presented above. We make the approximation:

$$\sqrt{t_i r_i} = a_3 p_{\infty}^{i-1} \tag{11}$$

so that:

$$r_i = \frac{a_3 p_{\infty}^{i-1}}{\left(1 - a_2^{i+1}\right)}$$
(12a)

$$t_i = a_3 p_{\infty}^{i-1} \left(1 - a_2^{i+1} \right)$$
(12b)

Equation 12b leads to a pair of Neumann series for relative transmittance:

$$T_{R,\lambda} = \frac{a_3\omega}{1 - p_\infty \omega} - \frac{a_3 a_2^2 \omega}{1 - p_\infty a_2 \omega}$$
(12c)

but no such series directly exists for relative reflectance. Instead, we must apply approximations to the reciprocal of $1-a_2^{i+1}$. One potential function for this is:

$$\frac{1}{1 - a_2^{i+1}} \approx 1 + a_4 a_5^{i-1} \tag{12d}$$

with

so:

$$a_4 = \frac{1}{1 - a_2^2} - 1 \tag{12e}$$

$$R_{R,\lambda} = \frac{a_3\omega}{1 - p_\infty \omega} + \frac{a_3 a_4 \omega}{1 - p_\infty a_5 \omega}$$
(12f)

As in the previous model, a_3 can be eliminated through consideration of energy conservation. The model technically now has one additional parameter, namely a_5 , although this too could be eliminated through further consideration of equation (12d).

The errors in model fitting are very similar to those shown in Figure 8, being slightly lower for higher LAI (at the cost of an additional model parameter). The fidelity in fitting the behaviour of the spectral invariants as a function of scattering order is also very similar.

4. DISCUSSION AND CONCLUSIONS

In this paper, we have examined a previous spectral invariant model of canopy directional-hemispherical reflectance and transmittance. We show that the model, based on assuming recollision probability to be constant with scattering order, is able to describe the required radiometric terms well for low to moderate LAI, but less well for higher LAI. The reason for this is seen to be that the model assumptions break down, and we see that the scattering behaviour as a function of interaction order is described by inappropriate functions. We proceed to examine the scattering terms in some detail as a function of ζ and other factors and see that the spectral invariants are generally well-behaved. If a better description of the spectral invariant functions could be formulated, such factors could be quite easily incorporated into the model. We do not explicitly examine bidirectional reflectance and transmittance terms here, but it is likely that these too could be easily modelled with similar concepts, most likely as a departure from the directional-hemispherical case.

From an examination of the square root of the ratio of escape probabilities, we propose a new formulation that, when combined with an assumption regarding the log-symmetry of the escape probabilities, leads to a numerical model of relative reflectance and transmittance. Whilst the operation of this model is good in regard to its ability to reconstruct scattering behaviour as a function of interaction order, the formulation does not directly lead to an analytical solution for reflectance and transmittance. We therefore apply a further approximation that permits this. The resulting model, expressed mainly through equations (12c) and (12f), performs as well or better than the full model, although as currently implemented this is at the cost of an additional model parameter.

The final analytical model is rather similar in form to the original model, in that it contains Neumann series. In place of the single series for total relative scattering however, we have three series, one of which governs scattering at high interaction orders and the other two, which contain functional equivalences, control the variation in escape and recollision probabilities at low orders of scattering.

The next directions for model development include using equation (12d) to eliminate the parameter a_5 , fully formulating for variations in zenith angle and ξ , and incorporating a treatment of bidirectional reflectance and transmittance. The model must also be nested within a fuller formulation incorporating interactions with the lower boundary. It is likely that for the black soil case the model parameters can be directly related to first-order reflectance and transmittance terms which can be analytically formulated for many cases. We can then consider the model to be essentially an improved description of multiple scattering in a canopy that is constrained by energy conservation, unlike many other formulations. The formulation appears to work reasonably well for the single heterogeneous canopy considered here, so it holds much promise as a general formulation. This should, however, be tested against a further range of conditions. Lewis and Disney (2007) showed that the original model could be applied to a description of leaf scattering, allowing for a convenient analytical nesting of this term as a function of pigment and other absorptances. Smolander and Stenberg (2005) showed that the original formulation allows for a nesting of multiple scales of clumping within a canopy. These concepts should also be further explored with the new formulation.

APPENDIX 1

MCRT simulations here are truncated at scattering order *i*=100. The sum of the scattering contributions $z = \sum_{i=100}^{i=100} s_i$ would equal

unity if this could be continued to infinity, from consideration of energy conservation. The term 1-z is due to scattering at interaction orders of greater than 100. Here, if 1-z is above a tolerance, further scattering orders are inferred, using the concept of recollision probability. Assuming p_{∞} to be constant after 100 interactions:

$$1 - z = s_{100} \sum_{i=1}^{i=\infty} p_{\infty}^{i} = s_{100} \frac{p_{\infty}}{(1 - p_{\infty})}$$
(A1)

so

$$p_{\infty} \approx (1-z)/(s_{100} + (1-z))$$
 (A2)

and further interactions estimated from $r_{i+1} = r_i p_{\infty}$ and $t_{i+1} = t_i p_{\infty}$. The maximum value of (1-z) is around 0.05 for LAI 20. It is clearly insignificant for low to moderate LAI.

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