A SPECTRAL INVARIANT APPROACH TO MODELLING RADIATIVE TRANSFER OF SUN-INDUCED CHLOROPHYLL FLUORESCENCE

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ABSTRACT

Sun-induced chlorophyll fluorescence (SIF) observations are strongly affected by canopy structure. Modelling the radiative transfer of SIF provides an approach to quantifying the canopy structure effects and a better estimation of photosynthesis from SIF. The spectral invariant approach allows for the separation of reflectance into spectrally dependent parameters and spectrally independent parameters. We extend the spectral invariant theory to model the radiative transfer of SIF. The spectral invariant approach gives similar simulations of SIF emission and scattering of far-red SIF as the SCOPE model does. This work can help to disentangle the part of SIF signal that is dependent on the structure from that which is dependent on physiology.

Index Terms— Sun-induced fluorescence, spectral invariant, canopy scattering, SCOPE, recollision probability

1. INTRODUCTION

Sun-induced fluorescence (SIF) is closely related to the light harvesting process of photosynthesis and responds dynamically to changes in photosynthesis. Its potential use as an actual photosynthetic activity allows early warning of vegetation stress conditions [1]. Temporally averaged satellite-based fluorescence data appear to correlate strongly with gross primary production (GPP) [2].

Physically linking SIF to photosynthesis is challenging. Canopy structure effects are one of the main obstacles for the interpretation of top-of-canopy (TOC) SIF measurements. Spatial or temporal variations of SIF measurements are regulated by canopy structure apart from photosynthetic functioning [3]. Emitted SIF by leaves interacts with the canopy and part of it is observed by a sensor at the top of the canopy. Understand the interaction between emitted SIF and vegetation canopies is essential to quantify the structural regulation on SIF signals, and thus obtain the direct functional status of photosynthetic mechanism.

Radiative transfer models (RTMs) are crucial tools to understand the canopy structural effects on SIF observations. Physically based RTMs requires the detailed parametrization of leaf properties and canopy structure. The spectral invariant theory quantifies canopy structure effects on canopy scattering, absorption by using a set of spectrally independent parameters. It may be useful for linking the structure effects on SIF observations and on reflectance.

In this study, we apply the spectral invariant theory in the radiative transfer of SIF and compare with a classic RTM (i.e., SCOPE [4]) for verification.

2. A SHORT REVIEW OF SPECTRAL INVARIANT THEORY

Photons coming from the top of a canopy will either go through the canopy via gaps directly or interact with phytoelements (leaves and needles). The portion of the photons from the incident beam that will interact with leaves is known as canopy interceptance (i_0). As a result of an interaction, photons can either be scattered or absorbed by a leaf, depending on the single scattering of the leaf. Leaf albedo (ω) taken as the sum of leaf reflectance (ρ) and transmittance (τ) describes the single scattering.

The scattered photons will either interact with phytoelements again or escape through the upper and lower boundary directly. The probability that a photon after having survived an interaction with a canopy element, will interact with the canopy again, is defined as the recollision probability (p) [5].

Canopy scattering for the incident radiation (s) is defined as the portion of the incident photons that will interact with phytoelements and escape through the upper or lower boundary after. Assuming that the recollision probability remains constant in successive interactions, canopy total scattering $s(\lambda)$ is computed [5] by using a geometric sequence:

$$s(\lambda) = i_0 \frac{(1-p)\omega(\lambda)}{1-p\omega(\lambda)} \tag{1}$$

Remote sensors typically measures the bidirectional reflectance factor (BRF) rather than total scattering. For the single direction illumination condition, it is defined as the ratio of observed radiance (L) times π to incident irradiance (E) (i.e., BRF = $\pi L/E$). The portion of scattered photons that escapes via gaps in the direction of observer (Ω_o) is the

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directional escape probability ($\rho(\Omega_o)$) [6, 7, 8]. BRF in the direction of observer is expressed as

$$\text{BRF}(\lambda) = i_0 \frac{\rho(\Omega_o)\omega(\lambda)}{1 - p\omega(\lambda)} \tag{2}$$

3. SIF EMISSION

Photons in the range of the photosynthetically active radiation (PAR) from 400 to 750 nm that hit the leaf, may excite fluorescence photons in the wavelength ranging from 640 to 850 nm. The excitation and emission relationship is described by a 350 by 211 matrix $\mathbf{M}(\lambda_e, \lambda_f)$. The fluorescence emission per unit of leaf area at a certain wavelength (λ_f) is excited by photons in the spectral region, and is expressed as:

$$E_F^l(\lambda_f) = \int_{400}^{750} \mathbf{M}(\lambda_f, \lambda_e) E(\lambda_e) d\lambda_e = \mathbf{M}E \tag{3}$$

The total fluorescence emission from the leaves is formed by all the interactions of PAR photons with the phytoelements. The fluorescence photons might excite fluorescence again, but this is negligible compared to the emission induced by scattered photons. One may assume that each leaf in the canopy has the same excitation-emission matrix $\mathbf{M}(\lambda_e, \lambda_f)$. The total SIF emitted by the leaves at a wavelength λ_f can be expressed as:

$$\begin{aligned} E_F(\lambda_f) =& \mathbf{M} i_0 [E + p\omega(\lambda_e)E + p^2\omega(\lambda_e)^2 E + ...] \\ =& \, i_0 \mathbf{M} E \frac{1}{1 - p\omega(\lambda_e)} \end{aligned} \tag{4}$$

4. SCATTERING OF EMITTED SIF

Canopy scattering for the emitted fluorescence (s_f) is defined as the portion of the emitted fluorescence photons by leaves that escapes through the boundaries. Once a fluorescence photon has been emitted, it may collide with the canopy depending only on the location of the emission event but not on the wavelength. Photons from a leaf after one interaction may interact with or escape from the canopy again regardless whether they are scattered or emitted. Thus, the canopy scattering of fluorescence $s_f(\lambda)$ can be also expressed by using the spectral invariants:

$$\begin{aligned} s_f(\lambda) =& (1-p) + p\omega(\lambda)(1-p) + p^2\omega(\lambda)^2(1-p) + ... \\ =& \frac{1-p}{1 - p\omega(\lambda)} \end{aligned} \tag{5}$$

Fluorescence observed by remote sensors is normally from one direction above the upper boundary of the canopy. We define the canopy directional fluorescence scattering (DFS, σ_{FC}) as the ratio of observed fluorescence radiance (L_F) times π to the total emitted fluorescence irradiance (E_F) by the leaves (i.e., $\sigma_{FC} = \pi L_F / E_F$). The canopy directional fluorescence scattering (DFS) can be expressed similarly to BRF [9].

$$\text{DFS}(\lambda) = \frac{\rho(\Omega_o)}{1 - p\omega(\lambda)} \tag{6}$$

5. LINKING SCATTERING OF SIF AND OF INCIDENT RADIATION

We obtain the relationship between canopy scattering of incident radiation from top of canopy and canopy scattering of emitted fluorescence by comparing Eq. 1 with Eq. 5.

$$i_0 \omega(\lambda) s_f(\lambda) = s(\lambda) \tag{7}$$

Similarly, we obtain the relationship between BRF and DFS by comparing Eq. 2 with Eq. 6.

$$i_0 \omega(\lambda) \text{DFS}(\lambda) = \text{BRF}(\lambda) \tag{8}$$

6. SIMULATION METHODS

Simulations from the SCOPE model were used to evaluate the spectral invariant theory in predicting canopy scattering of incident radiation and scattering of emitted SIF. BRF, DFS, the emitted SIF (E_F), s and s_f for 24 scenarios were modelled through SCOPE, and compared with prediction through the spectral invariant theory.

We examined 24 different canopy structures comprising all combinations of 4 LIDFs and 5 LAIs. Canopy LAI was set to from 1 to 6 with step 1, and four classes of leaf angle distribution of canopy were tested: planophile, erectophile, spherical, uniform. The solar zenith angle was 30° and the viewing zenith angle was 0°. Following the assumption of the spectral invariant theory that vegetation canopy is bounded by a non-reflecting surface, the soil reflectance was set to zero in the scenes of SCOPE simulation.

The spectral invariants for each scenario were obtained by fitting Eq. 1 and Eq. 2 for the SCOPE simulated leaf albedo and canopy observations. The canopy interceptance i_0 and recollision probability p were obtained by fitting Eq. 1. Further, the fitted parameters were used in the next step for retrieving the escape probability ($\rho(\Omega)$) by fitting Eq. 2. These three spectral invariants were later used to predict SIF emission, canopy scattering of SIF, and directional fluorescence scattering (DFS).

7. RESULTS

7.1. Simulation results of scattering and BRF

Spectral invariant theory gave nearly perfect prediction of canopy scattering of the incident radiation (Fig. 1A) and

BRF (Fig. 1B). The spectral invariant theory and SCOPE predicted almost the same canopy scattering and BRF for the 24 scenarios with R^2 = 0.997 and R^2 = 0.994 for s and BRF, respectively.

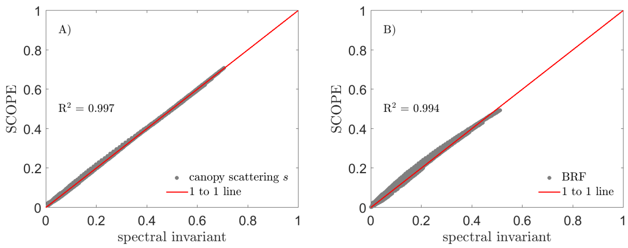

Fig. 1. Comparison of canopy scattering of the incident radiation s (A) and BRF (B) of the 24 scenarios predicted by SCOPE and by using spectral invariant theory.

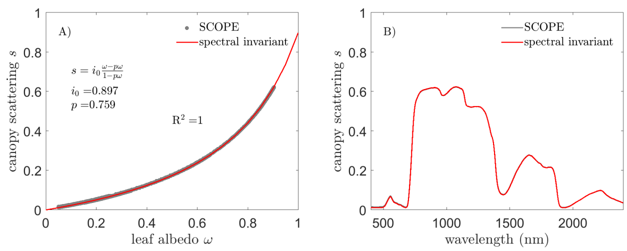

Fig. 2. A: Canopy scattering s versus leaf albedo ω from SCOPE and from the spectral invariant model for a canopy with LAI = 4 and with a spherical leaf inclination distribution; B: Spectra of canopy scattering predicted by SCOPE and by the spectral invariant theory for this canopy. Note: the spectral invariants of the canopy are fitting parameters. Canopy interceptance i_0 and recollision probability p, are 0.897 and 0.759, respectively.

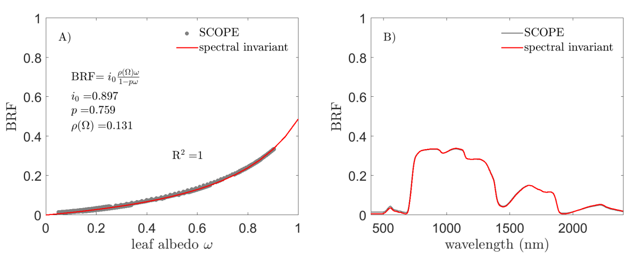

Fig. 3. A: BRF versus leaf albedo ω from SCOPE and from the spectral invariant model for a canopy with LAI = 4 and with a spherical leaf inclination distribution; B: Spectra of BRF predicted by SCOPE and by the spectral invariant theory for this canopy. Note: The canopy interceptance i_0=0.879, the recollision probability p= 0.759 and directional escape probability ρ= 0.131.

For the specific case (LAI = 4 and LIDF is spherical), the relationship between leaf albedo and canopy scattering of incident radiation and BRF was perfectly expressed by using the spectral invariants as shown in Eq. 1 and Eq. 2, respectively (Fig. 2 and Fig. 3). The disparity between the spectra simulated by SCOPE and by spectral invariant theory was minor. Only in the visible region, SCOPE predicted a slightly higher canopy scattering and BRF than the spectral invariant theory.

7.2. Simulation results of fluorescence

The spectral invariant theory and SCOPE simulated similar canopy fluorescence emission for the 24 scenarios (Fig. 4). Simulations results from SCOPE were slightly higher in the most cases. The spectra of fluorescence emission both from SCOPE and from spectral invariant theory peaked at 685 nm and 740 nm.

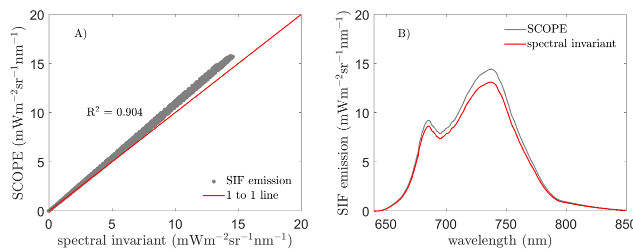

Fig. 4. A: Correlation of canopy total emitted fluorescence of the 24 scenarios predicted by SCOPE and by using spectral invariant theory; B: Canopy total emitted fluorescence predicted by SCOPE and by using spectral invariant theory for a canopy with LAI = 4 and with a spherical leaf inclination distribution.

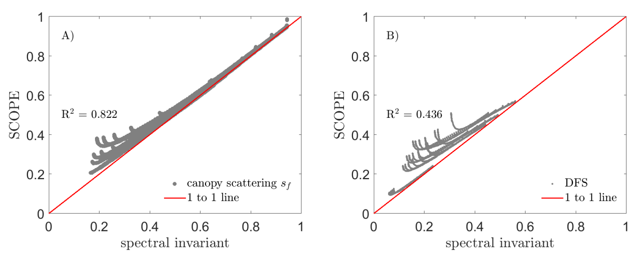

Fig. 5. Comparison of canopy scattering for the emitted SIF s_f (A) and DFS (B) predicted by SCOPE and by using spectral invariant theory. The spectra of s_f and DFS of the 24 scenarios predicted by SCOPE and by using spectral invariant theory are compared.

Canopy scattering of emitted fluorescence (s_f) and DFS from SCOPE and from the spectral invariant theory were comparable (Fig. 5). The simulation results of SCOPE and spectral invariant theory were similar when leaf albedo $\geq$ 0.5, but diverged for small leaf albedo. The two spectra matched in the near-infrared spectral region but not in the visible spectral region (Fig. 6 and Fig. 7). The spectral invariant theory predicted much different DFS in the visible spectral region compared with simulations from SCOPE.

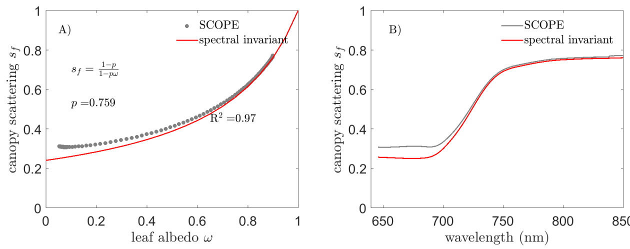

Fig. 6. A: Canopy scattering of SIF s_f versus leaf albedo ω from SCOPE and from the spectral invariant model for a canopy with LAI = 4 and with a spherical leaf inclination distribution; B: Spectra of canopy scattering predicted by SCOPE and by the spectral invariant theory for this canopy. Note: The canopy interceptance i_0=0.879, the recollision probability p= 0.759 and directional escape probability ρ= 0.131.

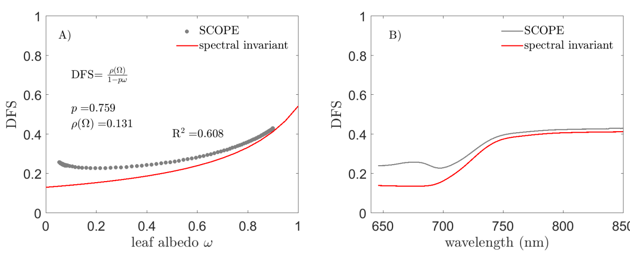

Fig. 7. A: DFS versus leaf albedo ω from SCOPE and from the spectral invariant model for a canopy with LAI = 4 and with a spherical leaf inclination distribution; B: Spectra of DFS predicted by SCOPE and by the spectral invariant theory for this canopy. Note: the spectral invariants of the canopy, recollision probability p= 0.759 and directional escape probability ρ= 0.131.

8. CONCLUSION

SIF scattering and reflectance have been linked by using the spectral invariant theory. It provides an opportunity to decouple canopy structure effects on SIF observations. The spectral invariant theory offers alternative approaches to predicting SIF emission and SIF scattering. Its use for these however requires several spectral invariants.

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