A SPECTRAL FITTING MODEL FOR CHLOROPHYLL FLUORESCENCE RETRIEVAL AT GLOBAL SCALE

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ABSTRACT

Chlorophyll sun-induced red and far-red fluorescence retrieval from space was recently proposed as a possible candidate for monitoring the vegetation status at global scale. Due to the very weak fluorescence emission signal in comparison to the reflected signal, detection is possible by performing radiance measurements in some of the atmospheric absorption bands where solar radiation is strongly attenuated while fluorescence is minimally influenced by this energy loss. To obtain an accurate retrieval of any information in the O_2A and O_2B absorption bands, we used high spectral resolution forward modeling and fitting. All the efforts were focused to determine the possibility of an accurate fluorescence retrieval at the VIS-NIR fluorescence Imaging Spectrometer (FIS) resolution (2 cm^{-1}) of the ESA FLEX mission [1]. In the case we present, we used MODTRAN5 at the maximum spectral resolution, i.e. 0.1 cm^{-1} for the radiation simulations and simulated fluorescence and reflectance at canopy level.

***Index Terms*—** High resolution, FLEX, Fluorescence, Vegetation

1. INTRODUCTION

For quantifying the influence of the impact of any transformation at global scale on vegetation, monitoring of chlorophyll fluorescence bands is necessary by means of an accurate retrieval process. Furthermore, canopy models are required to properly simulate the possible variations. Fluorescence retrieval is possible in the atmospheric absorption windows, for which a high resolution atmospheric modelling is required to fit any infilling component also smooth and slowly changing with wavelength. The radiance data collected in the two separate O_2A and O_2B absorption bands which represented in this case the observation spectral windows can be examined together if only one mathematical model is used for fluorescence, thus fulfilling the hyper-spectral monitoring concept. As any information even at low resolution from secondary instruments may be not available, careful measurements and retrieval performed on ground with the same algorithm become extremely useful for satellite monitoring not only for instrument calibration but also for the evaluation of those vegetation characteristics where the vegetation signal can be collected with minor atmospheric attenuation.

2. VEGETATION MODELS

For a demonstration of the fluorescence retrieval algorithm, we used simulated canopy fluorescence and reflectance obtained by means of a canopy fluorescence modelling set-up program (FluorSAIL) availing of a fluorescence-reflectance model at leaf level, which in turn is based on a model of leaf optical properties [2]. The program computed vertical profiles of the direct solar and the diffuse upward and downward fluxes inside the canopy by means of an analytic canopy radiative transfer subroutine by which it was possible to compute the total amount of light incident on leaves in the PAR region and to determine the fluorescence efficiency according to Rosema et al. [3]. The canopy in this case was characterized by a leaf area index (LAI) of 4 and a moderately erectophile leaf angle distribution [4].
According to these results, the direct solar flux spectrum changed only in level due to light interception by leaves, not in shape, while the diffuse downward flux changes also spectrally, from the sky irradiance spectral pattern at the top, to a typical green vegetation spectrum at the bottom. In this coupled model, four relevant reflectance terms were identified, two of which (i.e. r_{so} and r_{do}, the directional reflectance factors for solar and sky radiation, respectively) refer to the target, and two (i.e. $\overline{r_{sd}}$ and $\overline{r_{dd}}$, the hemispherical reflectance factors for solar and sky radiation, respectively) refer to the surroundings. In the retrieval of fluorescence, they were used to better evaluate the source of uncertainties resulting from the adjacency effects and the different scattering terms.

2. FUORESCENCE AND REFLECTANCE MATHEMATICAL MODELS

The two O_2B (shortly B) and O_2A (shortly A) spectral observation windows of FIS instrument are 20 nm wide and are nearby the red peak of the chlorophyll fluorescence band and the shoulder of the far-red one, respectively. The far red fluorescence peak is outside the A window. For monitoring the status of health of plants during their diurnal and seasonal evolution, a faithful reproduction of fluorescence within 10% error is required in the two spectral windows to assess the level of fluorescence emission. Also other sensible parameters like the ratio between the peaks in the two major emission bands would be desirable. In fact, the fluorescence peak intensities in the leaves undergo variations due to stresses and environmental changes that can be more sensitive than other variations. Hence, as a figure of merit of the mathematical model used for fluorescence fitting in the A and B spectral windows can be considered the possibility to deduce the ratio between the red and far red peak values with an uncertainty less than 10%. For example, polynomials are not suitable to give this joint information. These were used to fit fluorescence and reflectance in separated spectral regions. By fitting the FluorSAIL simulated fluorescence by means of the sum of two Voigt functions (8 parameters), it was possible to reach these goals, which were called the FIS requirements in the following. For the chosen FluorSAIL fluorescence simulation, the fitting with two Voigt functions was found more adequate than with two Gaussians, to which the two Voigts can easily reduce when other fluorescence simulations or "real" measurements would require that. The robustness of the algorithm was tested by adding a Gaussian noise to the simulated radiance proportional to the signal (GS) or to the square root of the signal (GSRS). In this procedure reflectance was fitted by means of cubic spline functions with a number of knots depending on the reflectance variation as a function of wavelength and the desired accuracy in fluorescence retrieval. The requirements on the fluorescence retrieval were assigned in terms of the Relative Root Mean Square Error % (RRMSE%) with respect to the magnitude of the observed value that was requested to be less than 10% in both A and B spectral windows.

3. RETRIEVAL ALGORITHM

For fluorescence retrieval we considered the general expression, given by Eq. 1, of the at-sensor radiance for a non-Lambertian target and surroundings in which the simulated hyperspectral multi-angular surface reflectance was deduced from the coupled soil-leaf-canopy and atmosphere radiative transfer modelling results [4]. Two series of 4 runs of MODTRAN5 were used covering both the O_2 absorption bands: 677nm – 697nm and 750nm – 770nm with a nadir viewing sensor situated at 800 km above a ground altitude of 200m and at the top of the canopy for TOA and BOA simulations, respectively. The sun was at a zenith angle of 30°, a rural aerosol type and a mid-latitude summer atmosphere were selected. The visibility was 23 km. In Eq. 1, the simulated canopy fluorescence and reflectance terms for both direct and diffuse radiation were re-sampled at the resolution of MODTRAN 5.

$$L_o = t_1 + t_2 F + t_4 r_{so} + \frac{t_5 + t_6 \overline{r_{sd}}}{(1 - t_3 \overline{r_{dd}})} r_{do} + \frac{t_7 \overline{r_{sd}} + t_8 \overline{r_{dd}}}{1 - t_3 \overline{r_{dd}}} \quad (1)$$

In Eq. (1) t_1 is the atmospheric (black earth) path radiance, t_2 is the target-sensor transmittance, t_3 is the spherical albedo of the bottom of the atmosphere, and t_4 and t_8 are several radiance terms (in the same units as t_1 and F). The terms t_1-t_8 were extracted by a MODTRAN5 Interrogation Technique (MIT) [4], based on the 4 runs. The outputs were obtained for the maximum MODTRAN5 resolution, i.e. 0.1 cm^{-1} and comprised about 7700 data points. Spectral radiances were expressed in W/cm^2-sr-cm^{-1}. In this analysis, we first adopted the scheme of retrieving fluorescence and a unique reflectance R for comparison with the Lambertian surface case. Furthermore, by coupling the reflectance terms according to their origin, we retrieved fluorescence and the vegetated target reflectance Rt which was one of the two weighted reflectances, and evaluated the surrounding effects by means of the other one (Ra). This second cycle utilized the previous fitting results and enhanced the accuracy of the fluorescence retrieval.

The sensor radiance (SENSOR_RAD) at TOA or at canopy level was obtained from the convolution of the total radiance with the Instrumental Line Shape (ILS) of the detection instrument as:

$$\text{SENSOR\_RAD} = [\, L_o \,] \otimes \text{ILS} \quad (2)$$

where ⊗ indicates the operation of convolution. In the absence of measurements, *F* and r_i (*i = so, do, sd, dd*) are the simulated data and ILS is a Gaussian function whose FWHM was changed in a range between 0.47 to 47 cm^{-1}. For the retrieval, $SENSOR\_RAD_m$ was used generated by inserting in (2) the mathematical functions F_m, r_m, and ILS_m that represented the unknowns in place of the simulated values. After resampling of the signals from the MODTRAN5 minimum sampling (0.1 cm^{-1}) to that of a simulated instrument, Equation (2) reduced to a set of n equations, one for each sampled value of SENSOR_RAD (n = 454 for the FIS sampling equal to 1.7 cm^{-1}, for example). Gaussian noise was added to this term to model the behavior of the sensor. Residuals RES were defined as:

$$RES\% = 100 \times DS / SENSOR\_RAD_{max} \quad (3)$$

where DS is equal to the difference ($SENSOR\_RAD_n$- $SENSOR\_RAD_m$) between the simulated with noise and the retrieved sensor radiance, and $SENSOR\_RAD_{max}$ is the maximum value of SENSOR_RAD in the two FIS windows. LSQCURVEFIT is the Least Square Program of MATLAB7 that minimized the residuals to find the set of parameter values for F_m, r_m, and ILS_m in $SENSOR\_RAD_m$ by means of a best fit procedure depending on the mathematical model adopted. The retrieval algorithm and fitting process evaluated all the equations. Moreover, all the data were divided by SENSOR_RAD itself to facilitate the minimization procedure. The Relative Root Mean Square Error (RRMSE%) with respect to the magnitude of the observed value in conjunction with residuals were used for the evaluation of the results.
The influence of noise statistics on fluorescence RRMSE% was also analyzed by repeating the procedure and recording the spread of values with respect to the mean value obtained in a cycle of successive minimizations.

4. RESULTS

In the following we report the results obtained at TOA for different resolutions and samplings which were scaled according to the resolution value. In particular, we report the results obtained at a resolution of 4.7 cm^{-1} and a sampling of 1.7 cm^{-1} that safely overestimate the consequences of a binning between pixels for the FIS sensor. Fluorescence retrieval from space is more difficult than on-ground as transmitted fluorescence signal is only a minor part of the sensor radiance, and scattering effects, which are almost absent on ground, represent a substantial part of the sensor radiance at TOA. For the fluorescence examined case, the ratio of the fluorescence peak values: peak[A]/peak[B] turned out to be equal to 1.13 and the maximum of fluorescence Fmax was equal to 1.24×10^{-8} W/cm^2 sr cm^{-1}.
Before performing the retrieval of fluorescence and reflectance terms, we first performed a retrieval of fluorescence by using no noise in SENSOR_RAD and all the simulated reflectances in place of the reflectance mathematical functions in $SENSOR\_RAD_m$. This allowed us to find the best values for the Voigt parameters, and to deduce the value k of the ratio between the intensities of the two fluorescence Voigts.
When noise was added and reflectance retrieved along with fluorescence, the retrieval at TOA fulfilled the requirements proposed for the FIS instrument (accuracy in fluorescence retrieval better than 10%) associated to an error of the "measurement" (RRMSE% of noise) less than 0.22% (0.27%) for a GS (GSRS) type noise. At canopy level the same FIS requirement could be satisfied with a larger than about two times error. We considered these values as a limit for the retrieval of real measurements at TOA. It was imposed mainly by the spread inherent in the noise statistics. The rms value N of the difference between sensor radiance with and without noise in each band:

$$N = rms\,(SENSOR\_RAD - SENSOR\_RAD_n) \quad (4)$$

can be utilized for an evaluation of the instrument SNR. In Fig.1, SENSOR_RAD/N is shown for the GSRS (photon-noise limited case) maximum RRMSE% value used in the A band.

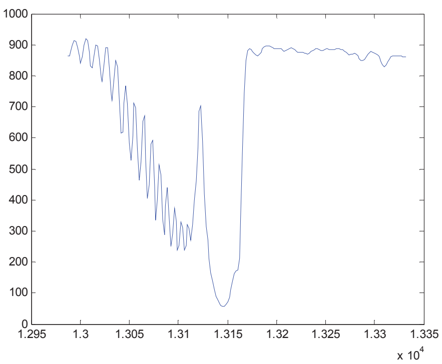

Figure 1. SENSOR_RAD/N as a function of wavenumbers in the A band for a GSRS noise of RRMSE%=0.27.

For the same maximum value, SENSOR_RAD/N was extending in the B spectral window from a minimum of 170 in the main absorption band to a maximum of 400 in correspondence of the low frequency limit.
For the retrieval we used up to {15, 15} nodes for R in the unique reflectance case, where the first and the second numbers in parenthesis refer to A and B windows, respectively. Furthermore, for the coupled reflectances retrieval case, we used up to {3,12} and {2,12} knots for Rt for Ra in the *bare* case, respectively, while in the *same* case up to {12,12} knots in both windows. With a high number of knots the fitting procedure can be properly controlled by lowering the optimization tolerances. The largest number of knots corresponded to uniformly distributed frequency samples of about 1.5 nm in width, a range value which was utilized when fitting with polynomials for obtaining the required accuracy on ground. The fitting was performed also assuming an instrument resolution comparable to the MODTRAN5 maximum resolution. The accuracy in fluorescence retrieval resulted improved by a factor two, and the fitting cycle reduced to a single run of about 10 step. When decreasing the resolution, additional cycles are necessary. The method could be successfully employed up to a maximum resolution of about 9.4 cm^{-1}. For still lower resolutions than that, fluorescence resulted overestimated.

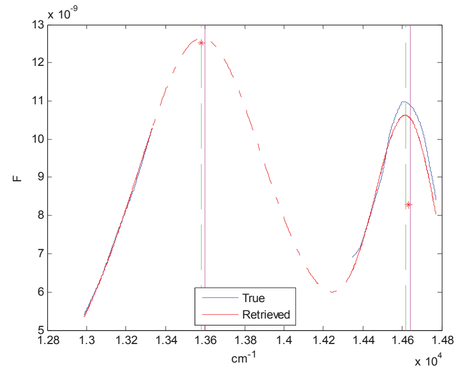

Figure 2. Simulated and retrieved fluorescences (*same* case) in the two A and B bands for a GSRS noise of RRMSE% = 0.27. The asterisks indicate the intensities and positions of each Voigt in the variability position range indicated by means of the vertical lines.

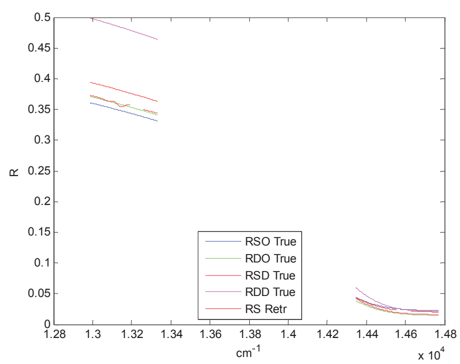

Figure 3. R retrieved reflectance and simulated reflectances in the two A and B bands for a GSRS noise of RRMSE% = 0.27 in the *same* case. R resulted very close to *rso*.

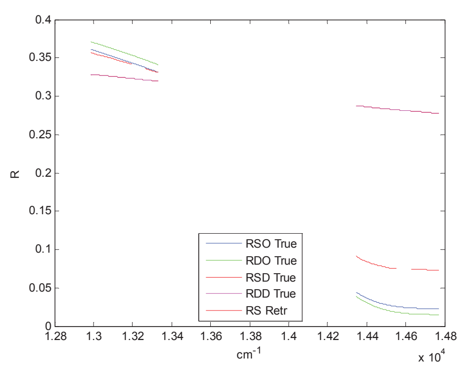

Figure 4. R retrieved reflectance and simulated reflectances in the two A and B bands for a GSRS noise of RRMSE% = 0.27 in the *bare* case. Valuable is the difference between R and *rso* in the B band.

5. CONCLUSIONS

The possibility of an accurate fluorescence retrieval was tested at resolutions extending in a range which cover existing or planned sensor instruments characteristics for fluorescence retrieval on ground and for other molecular species detection from space. The study was performed in the atmospheric A and B absorption bands of molecular oxygen where high resolution methods are necessary for the retrieval of also slowly varying signals with wavelengths. A simulated canopy fluorescence and four associated reflectances were used. The importance of a spectroscopic function for fitting fluorescence was also assessed. For the fluorescence retrieval from space, an accurate study on ground would be useful with an instrument which had the same resolution of FIS. All the information on fluorescence that can be deduced from other methods can enrich the initial guess data set for fluorescence retrieval in optimized conditions.

6. REFERENCES

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