RADIATIVE MODELING AND CHARACTERIZATION OF AEROSOL PLUMES IN HYPERSONTICAL IMAGERY

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ABSTRACT

A semianalytical model, named APOM (Aerosol Plume Optical Model) and predicting the radiative effects of aerosol plumes in the spectral range [0.4,2.5 μm], is presented in the case of nadir viewing. The scene is represented by an atmospheric layer (molecules and natural aerosols) located above the plume layer. The estimated at-sensor reflectance depends on the solar zenith angle, the plume optical properties (optical depth, single-scattering albedo and asymmetry parameter), the ground reflectance and the wavelength. Its numerical coefficients are derived from COMANCHE radiative transfer simulations. Model accuracy is assessed by using a set of simulations performed in the case of biomass burning and industrial plumes. APOM proves to be accurate and robust for solar zenith angles between 0° and 60° whatever the sensor altitude, the standard atmosphere and for plume phase functions defined from urban and rural models. The modeling errors in the at-sensor reflectance are on average below 0.002. They can reach values as high as 0.01 for wavelengths close to 0.4 μm but mainly correspond in such cases to low relative errors (below 5% and 3% on average). This model can be used for forward modeling (quick simulations of multi/hyperspectral images, help in sensor design...) as well as for the retrieval of the plume optical properties. For this purpose, we propose a model for the optical properties involving a few parameters and we show that even in this case the problem is still ill-constrained and that constraints have to be imposed. First retrieval results as well as recommendations for the inversion are presented.

INTRODUCTION

Understanding the impact of aerosols on climate and on human health is a field of research that still requires new developments (i). Aerosols are liquid and solid particles suspended in the atmosphere that originate from natural or man-made sources of emission. They can reflect and absorb solar radiation (the aerosol direct effect) and modify cloud properties (the aerosol indirect effect) (ii). These phenomena are very variable depending on sources of emission, which makes difficult the assessment of the aerosol impact on the radiative budget (ii).

Remote sensing methods are well suited for aerosol characterization. They generally make use of a few wavelengths (iii,iv), multiangle (v,vi) and polarization information (vii). In order to better understand the global effect of aerosols, it is necessary to characterize the local sources of emission (viii). In this study, we are focusing on smoke plumes which result from local high emission events, like biomass burning plumes and industrial plumes. Studies on pollution and climate are using models on particles circulation which are valid at a global scale (viii). These models require local data as references. This paper aims at characterizing
the local sources of aerosols and then contributes to providing such data. Moreover, it would help in understanding the spatial distribution of natural and anthropogenic aerosols.

In this paper, a semianalytical model of the spectral signal (at-sensor reflectance) above plumes in the spectral range [0.4, 2.5 \( \mu m \)] is proposed. Multiple scattering plays a great role in the case of dense plumes. It can be accurately computed by using algorithms like DISORT (ix) (DIScrete Ordinates Radiative Transfer) but unfortunately this operation is very time consuming. Disposing of a semianalytical model which would take into account multiple scattering would then be a fruitful advance in the purpose of forward modeling but also in the purpose of retrieval. Indeed, the usual techniques in signal processing could be used to invert the optical properties from the model (deterministic or stochastic methods). Moreover, it may provide more accurate results than existing methods which mainly rely on look-up tables.

Then, the outline of this paper is the following. In a first step, the plume signal is modeled as a function of the optical properties of aerosols (optical depth, single-scattering albedo, asymmetry parameter), the viewing conditions (solar zenith angle, sensor is at nadir) and the ground reflectance. It yields a semianalytical model named APOM (Aerosol Plume Optical Model) whose accuracy and robustness are assessed by using a large database of optical properties. In a second step, each optical property is modeled by using a few parameters. Then, in a third step, first retrieval results as well as recommendations for the inversion are presented.

1 DESCRIPTION OF THE APOM MODEL

In this section, we first present the theoretical description of APOM. Afterwards, the algorithm and data used to derive its numerical coefficients are presented. Finally, the APOM accuracy and robustness are discussed. For a detailed description of the model, see Alakian et al. (x).

1.1 ANALYTICAL FORMULATION

Considering a plane-parallel atmosphere, the at-sensor radiance is the result of photons coming from the landscape and the atmosphere. The at-sensor reflectance \( \rho_{\text{sensor}} \) is defined here as

\[
\rho_{\text{sensor}} = \frac{\pi L_{\text{sensor}}}{\mu_s E_s}
\]

where \( L_{\text{sensor}} \) is the at-sensor radiance, \( \mu_s \) is the cosine of the solar zenith angle \( \theta_s \) and \( E_s \) is the extraterrestrial solar irradiance. Considering reflectance rather than radiance allows to overcome variations of sun irradiance and sun geometry. This notation is used whatever the altitude of the sensor which can be either airborne or satelliteborne. Assuming a homogeneous lambertian surface with a reflectance \( \rho \), \( \rho_{\text{sensor}} \) can be expressed as (xi)

\[
\rho_{\text{sensor}} = \rho_{\text{atm}} + \frac{T_{\text{atm}} \rho}{1 - S_{\text{atm}}}
\]

where \( \rho_{\text{atm}} \) is the upwelling atmospheric reflectance, \( T_{\text{atm}} \) is the total transmittance (direct and diffuse) of the atmosphere along the sun-ground-sensor path and \( S_{\text{atm}} \) is the atmospheric spherical albedo. Wavelength dependency of each term has been omitted for clarity.

Let us consider a homogeneous aerosol plume added in a layer just above the ground. The atmospheric terms \( \rho_{\text{atm}}, T_{\text{atm}} \) and \( S_{\text{atm}} \) are then modified by the presence of the plume. APOM
assumes that each atmospheric term can be expressed as the combination of two terms: a first one which is the corresponding atmospheric term for the same scene without plume and a second one due to the plume (see Fig. 1). APOM proposes to model \( \rho_{\text{atm}}, T_{\text{atm}} \) and \( S_{\text{atm}} \) for a nadir viewing sensor as functions of the plume optical properties (fully characterized by the optical depth \( \tau \), the single-scattering albedo \( \omega_0 \) and the asymmetry parameter \( g \)) and the solar zenith angle. At a given wavelength, \( \rho_{\text{atm}}, T_{\text{atm}}, S_{\text{atm}} \) are modeled with the following expressions:

\[
\rho_{\text{atm}}(\tau, \omega_0, g, \mu_s) = \rho_{0,\text{atm}}(\mu_s) + \sum_{(i,j) \in I} m_{ij} \omega_0 g^j \left[ 1 - \exp\left( \sum_{(i,j,k) \in I \times J \times K} (n_{ijk} + p_{ijk} \mu_s^k) \tau^k \omega_0^j g^j \right) \right]
\]

\[
T_{\text{atm}}(\tau, \omega_0, g, \mu_s) = T_{0,\text{atm}}(\mu_s) \exp\left( \sum_{(i,j,k) \in I \times J \times K} (q_{ijk} + r_{ijk} \mu_s^k) \tau^k \omega_0^j g^j \right)
\]

\[
S_{\text{atm}}(\tau, \omega_0, g, \mu_s) = S_{0,\text{atm}} + \sum_{(i,j) \in I \times J} s_{ij} \omega_0 g^j \left[ 1 - \exp\left( \sum_{(i,j,k) \in I \times J \times K} t_{ijk} \tau^k \omega_0^j g^j \right) \right]
\]

where \( \rho_{0,\text{atm}}, T_{0,\text{atm}} \) and \( S_{0,\text{atm}} \) are respectively the upwelling atmospheric reflectance, the total transmittance and the atmospheric spherical albedo in the case of a given atmosphere without plume. \( I = \{0,1,2,3,4\}, J = \{0,1,2,3\}, K = \{1,2,3\}. \) \( m_{ij} \), \( n_{ijk} \), \( p_{ijk} \), \( q_{ijk} \), \( r_{ijk} \), \( s_{ij} \), \( t_{ijk} \) are the fitting coefficients.

These considerations have been made for one wavelength. Modifying the wavelength does not change the shape of \( \rho_{\text{atm}}, T_{\text{atm}}, S_{\text{atm}} \) but the fitting coefficients are different. This is due to a coupling (xii) between the aerosol plume and the molecules from the standard atmosphere. This coupling is due to Rayleigh scattering (important for the shorter wavelengths) and to the numerous gaseous absorption lines along the spectrum. Then the fitting coefficients are calculated for each wavelength separately. Unfortunately, it seems that it is not possible to model each coefficient as a simple function of wavelength.

**Figure 1: APOM principle.** At-sensor atmospheric terms \( (\rho_{\text{atm}}, T_{\text{atm}}, S_{\text{atm}}) \) are modeled as combinations of standard atmospheric terms \( (\rho_{0,\text{atm}}, T_{0,\text{atm}}, S_{0,\text{atm}}) \) and plume atmospheric terms \( (\rho_{\text{plume}}, T_{\text{plume}}, S_{\text{plume}}) \). Standard terms are computed by considering the scene without plume.
and by taking into account gases and natural aerosol profiles from ground to sensor. Plume terms are computed from APOM coefficients.

1.2 ESTIMATION OF THE MODEL COEFFICIENTS

In order to determine the fitting coefficients, a set of simulations has been conducted by varying the optical properties of the plume, the wavelength and the solar zenith angle. In this purpose, the radiative transfer code COMANCHE (xiii) based on a MODTRAN4 kernel (xiv) is used. The optical depth $\tau$ can take values in the set $\{0.0,0.1,0.2,0.4,0.6,0.8,1.0,1.3,1.6,2.0,2.4,2.8,3.2\}$. The single-scattering albedo $\omega_0$ takes its values in the set $\{0.00,0.45,0.60,0.69,0.77,0.84,0.90,0.95,0.98\}$. Values of the asymmetry parameter $g$ belong to $\{0.01,0.10,0.20,0.30,0.45,0.60,0.75,0.90\}$. Ranges are defined from available data on plumes. These sets have been established by studying the impact of each parameter: simulations show that this impact increases faster and faster as $\omega_0$ increases and $\tau$ and $g$ decrease, which explains the variable steps used for each set. For wavelength, all the computations are made on 15 cm$^{-1}$ wavelength grid in the range [0.4,2.5$\mu$m]. The solar zenith angles $\theta_s$ are chosen in the set $\{15^\circ, 30^\circ, 45^\circ, 60^\circ\}$. The fitting coefficients are determined from all the combinations of these simulations by minimizing the modeling error in the sense of the root mean square.

The presented model has been computed with a spectral resolution of 15 cm$^{-1}$. Such a resolution is sufficient for a future use with hyperspectral sensors which have resolutions of about 10 nm in the spectral range [0.4,2.5$\mu$m]. If one requires to use the model for a particular sensor, coefficients that are adapted to its spectral bands are required. Then, for a given sensor, all the computations performed so far with COMANCHE have to be convolved with the normalized spectral response. The method described before is then applied to determine the model coefficients. In the example of the hyperspectral sensor AVIRIS (Airborne Visible/InfraRed Imaging Spectrometer (xv), 224 bands), the plume signal measured by this sensor can be modeled with 64736 coefficients (224 bands $\times$ 289 coefficients). Note that once the database of simulations has been computed at 15 cm$^{-1}$, the model coefficients corresponding to a given sensor are determined fastly and can be used for all images from this sensor.

1.3 VALIDATION OF APOM

A large set of simulations has been performed in the case of biomass burning and industrial plumes in order to validate the model. The model proves to be accurate for solar zenith angles between 0$^\circ$ and 60$^\circ$. The modeling errors are on average below 0.002 in $\rho_{\text{sensor}}$. Errors can reach values as high as 0.01 for wavelengths close to 0.4 $\mu$m, but these errors mainly correspond to low relative errors (below 5%). The model preserves its accuracy whatever the sensor altitude and the standard atmospheric model. APOM proves also to be robust when natural aerosols are added in the atmosphere. All these assessments are fully described in Alakian et al. (x).

The APOM coefficients computed over all the wavelengths of interest allow to generate quasi-instantaneously $\rho_{\text{sensor}}$ within [0.4,2.5$\mu$m] whatever the plume optical properties $\tau$, $\omega_0$, and $g$ and whatever the solar zenith angle $\theta_s$. To give an idea about the gain in time, the simulation of one pixel with COMANCHE at AVIRIS spectral resolution with given optical properties requires about one hour with current computers (e.g. AMD Opteron 2.40 GHz) whereas only a few milliseconds are required by using APOM. Note that the model only depends on $\tau$, $\omega_0$ and $g$, then the model is fully general (for aerosol plumes with $g>0$).
2 MODELING OF THE PLUME SPECTRAL OPTICAL PROPERTIES

In order to be used for inversion, APOM requires the plume spectral optical properties as inputs. Assuming sphericity and homogeneity of particles as well as their complex refraction index and their size distribution, Mie theory (xvi) allows one to compute the optical properties of aerosols. Unfortunately, the resulting expressions are quite complex and then cannot be used easily to develop a retrieval method. As aerosols exhibit slow spectral variations, we propose to model the spectral dependency of the optical properties with a few parameters.

Usually, the aerosol optical thickness is assumed to follow the Angström (xvii) law 
\[ \tau = \beta \lambda^{-\alpha} \]
where \( \lambda \) is the wavelength (in \( \mu \)m), \( \beta \) the Angström turbidity coefficient, and \( \alpha \) the Angström wavelength exponent. Actually, it models \( \ln \tau \) with a straight line as a function of \( \ln \lambda \). Typical values for \( \alpha \) range from >2 for fresh smoke aerosols to nearly zero for Sahelian/Saharan desert dust cases dominated by coarse mode aerosols (xviii). This law provides good results for aerosol size distributions following a Junge power. But in real cases, \( \ln \tau \) has often a curvature that cannot be modeled with Angström law. Then King and Byrne (xix) utilized a second-order polynomial fit to account for the curvature of \( \ln \tau \) as 
\[ \ln \tau(\lambda) = a_0 + a_1 \ln \lambda + a_2 \ln^2 \lambda . \]
We propose to generalize this formulation by
\[ \tau(\lambda) = \exp \left( \sum_{j=0}^{M_\tau-1} a_j \ln^j \lambda \right) \]
where the \( a_j \) are the parameters to be estimated and \( M_\tau \) is the number of parameters. In the same manner, as the single-scattering albedo is a slowly varying function of wavelength, a similar formulation is proposed
\[ \omega_0(\lambda) = \exp \left( \sum_{j=0}^{M_\omega-1} b_j \ln^j \lambda \right) \]
where the \( b_j \) are the parameters to be estimated and \( M_\omega \) is the number of parameters. The asymmetry parameter \( g \) is modeled as follows
\[ g(\lambda) = \sum_{j=0}^{M_g-1} c_j \lambda^j \]
where the \( c_j \) are the parameters to be estimated and \( M_g \) is the number of parameters.

Heavy aerosol plumes mostly contain small particles that can be observed for wavelengths below 1 \( \mu \)m. Above such wavelengths, the impact of aerosols on the radiance measured by a remote sensor can hardly be differentiated from the ground impact. By restraining the spectral range to \([0.4,1.1\mu\text{m}]\) for which the aerosol impact is maximum, Alakian et al. (xx) have shown that modeling \( \tau(\lambda) \) with three parameters \( (a_0, a_1, a_2) \), \( \omega_0(\lambda) \) with three parameters \( (b_0, b_1, b_2) \) and \( g(\lambda) \) with two parameters \( (c_0, c_1) \) provides quite accurate results (see Fig. 2). An assessment of the fitting accuracy has been performed by using large sets of optical properties for biomass burning and industrial particles and proves that such a modeling leads to an overall root mean square error below 0.005 for each optical property.
Figure 2: Modeling $\tau(\lambda)$, $\omega(\lambda)$ and $g(\lambda)$ for biomass burning plume particles, composed of 10% of black carbon and 90% of organic carbon and with monomodal lognormal size distribution (modal radius of 0.1 µm and standard deviation of 1.35). Using three parameters for $\tau(\lambda)$ and $\omega(\lambda)$ and two parameters for $g(\lambda)$ provides accurate fits (root mean square error below 0.005 for each optical property).

3 USE OF APOM FOR CHARACTERIZATION OF AEROSOL PLUMES

3.1 PRINCIPLE OF RETRIEVAL

The model APOM and the modeling of the spectral optical properties enable to characterize the at-sensor reflectance $\rho_{\text{sensor}}$ from the plume parameters $a_0$, $a_1$, $a_2$, $b_0$, $b_1$, $b_2$, $c_0$ and $c_1$ (unknown), the cosine of the solar zenith angle $\mu_s$ (known), the sensor spectral bands $\lambda$ (known) and the ground reflectance $\rho_\text{atm}$ (a priori unknown):

$$\rho_{\text{sensor}}(\lambda) = f(a_0, a_1, a_2, b_0, b_1, b_2, c_0, c_1, \mu_s, \lambda, \rho(\lambda))$$

where $f$ is a function defined by the joint use of APOM and the modeling of the spectral optical properties. If the ground is assumed to be known, only the aerosol parameters need to be estimated (eight unknowns). As each spectral band provides an equation between these parameters, at least eight bands are theoretically needed to perform the retrieval. Hyperspectral sensors provide tens or hundreds of bands and then fit this requirement. Retrieval of $a_0$, $a_1$, $a_2$, $b_0$, $b_1$, $b_2$, $c_0$ and $c_1$ is performed by minimizing the least squares between observed and modeled $\rho_{\text{sensor}}$ with a Generalized Reduced Gradient Method.

3.2 FIRST RESULTS AND CLUES

This study focuses on a hyperspectral image from the Quinault biomass burning plume that were acquired with AVIRIS during the Sulfate, Clouds And Radiation (SCAR) field experiment in the summer of 1994 in the state of Washington (47.32 N, 124.27 W, AVIRIS 092194, run 10, scene 1, flight altitude: 20 km). The motivation of this choice is twofold: at first, the plume is located above the ocean (low reflectance) and then the at-sensor reflectance is largely due to the atmospheric reflectance ($\rho_{\text{sensor}} \approx \rho_{\text{atm}}$), secondly optical and microphysical measures have been performed in situ and then can be used for comparison with the retrieval results. Then, in this study, we assume that $\rho_{\text{sensor}} = \rho_{\text{atm}}$. Before being used for inversion, APOM requires $\rho_{\text{atm}}$ as input. $\rho_{\text{atm}}$ can be computed from the image by averaging the reflectance of the water pixels located outside the plume (i.e. $\rho_{\text{sensor}} = \rho_{\text{atm}}$ outside the plume).

In order to make easier the retrieval, a database of biomass burning plume optical properties is used to restrain the variation ranges of the aerosol parameters.
The inversion of the Quinault image is presented here. Inversion of several pixels from the plume is performed. The retrieved optical properties (computed from the retrieved $a_0$, $a_1$, $a_2$, $b_0$, $b_1$, $b_2$, $c_0$, $c_1$) can have very variable spectra as it will be discussed later. To have comparable results, we assume the plume is quite homogeneous, its composition and size distribution do not change much from one pixel to one another. Then, we consider that the parameters $c_0$ and $c_1$ (i.e. $g$) are the same for every pixel: from several simulations we chose $c_0 = 0.52$ and $c_1 = -0.3$. The inversion of every pixel from the image is presented in Fig. 3. Maps in optical depth seem to be correlated to the image: the brighter the pixels, the more concentrated in aerosols the pixel is and the higher the optical depth. However, the maps in single-scattering albedo show that particles are all the more diffusing than they are less concentrated, which has no physical signification.

Figure 3: a) Quinault image at 550 nm, b) image and retrieved at-sensor reflectance for the white cross pixel, c) retrieved optical properties for the white cross pixel, d) maps of retrieved $\tau$ values at 550 nm, 800 nm and 1100 nm, e) maps of retrieved $\omega_0$ values at 550 nm, 800 nm and 1100 nm.

Then, inversing the aerosol parameters without imposing any more constraint can lead to inexact results. Indeed, it is possible that different triplets of optical properties ($\tau(\lambda)$, $\omega_0(\lambda)$, $g(\lambda)$) lead to the same at-sensor reflectance, as illustrated in Fig. 4. The plume pixel can be reproduced with three different triplets. Retrieval is then an ill-constrained problem. Additional constraints are required to suppress the wrong triplets. Several approaches are investigated.
First of all, a sensitivity study on the aerosol parameters must be led in order to determine which ones have the bigger impact and then are likely to be inverted. Such a study could also show that only combinations of parameters could be retrieved. For example, $a_0$ and $b_0$ may not be inverted separately but their product $a_0b_0$ may be.

Adding some information on the optical properties interdependency can bring some strong constraints. Indeed, any triplet $(\tau(\lambda), \omega_0(\lambda), g(\lambda))$ may not have a physical signification. The analysis of the database on biomass burning plume optical properties show that some information redundancy exist between the optical properties of a same triplet. Some first results show that it is possible to strongly constraint the variation ranges of $c_0$ and $c_1$ from the knowledge of $a_0$, $a_1$, $b_0$, $b_1$ and $b_2$. Such an approach would surely suppress most of unfeasible solutions.

Another approach is to exploit the spatial dimension of image by searching for the denser parts of the plume. The interest is twofold. On one hand, it is not necessary to care about the ground reflectance located under the plume because photons are all absorbed or scattered and then never reach it ($\rho_{\text{sensor}} = \rho_{\text{atm}}$). On another hand, $\rho_{\text{sensor}}$ is little sensitive to optical depth $\tau$ when this one is high. When $\tau$ increases, $\rho_{\text{atm}}$ converges towards asymptotic value (see third equation) which only depends on $\omega_0(\lambda)$ and $g(\lambda)$. Then, in dense parts, only five aerosol parameters (instead of eight) are needed to be retrieved. The estimated parameters could be used to extrapolate the corresponding parameters in the less dense parts ($\omega_0(\lambda)$ and $g(\lambda)$ are assumed not to change a lot from one pixel to another).

Finally, the ground reflectance $\rho$ located under the less dense parts of the plume should also be estimated because its impact on $\rho_{\text{sensor}}$ cannot be neglected. In this purpose, we propose to study the wavelengths where the plume is completely transparent (e.g. $\lambda > 1.4\mu m$) and to extrapolate $\rho$ to other wavelengths ($\lambda < 1.4\mu m$) by performing correlations with the pixels outside the plume.

Figure 4: Illustration of the non unicity of the solutions during inversion. a) At-sensor reflectance (black line) can be reproduced with several triplets $(\tau(\lambda), \omega_0(\lambda), g(\lambda))$ (blue, green and red lines) for which spectral behaviour is represented in b), c) and d).
4 CONCLUSION AND DISCUSSION

The semianalytical forward model APOM for the radiative effects of optically thick aerosol plumes in the spectral range [0.4,2.5µm] has been presented in the case of nadir viewing. The model is modular and may be improved by including the sensor direction (zenith and azimuth angles) as a parameter. Then, it could be used for multiangle imaging sensors. This model allows fast simulations of multi/hyperspectral images of plumes, to study the aerosol radiative impact (climate...), to assess the sensitivity of the at-sensor signal to the aerosol properties or to help in sensor design.

For retrieval, the generation of huge look-up tables is now possible very quickly with a high accuracy (DISORT 16 fluxes accuracy). It is also possible to develop more accurate methods of retrieval by adapting the existing methods in signal processing which use analytical models (gradient descents, ...). A modeling of the spectral optical properties with a few parameters is proposed and we show how it can be jointly used with APOM for inversion. First results are presented and reveal that constraints have to be imposed. For this purpose, several clues are considered.

REFERENCES


