Journal of Quantitative Spectroscopy & Radiative Transfer 192 (2017) 14–29

Contents lists available at ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

journal homepage: www.elsevier.com/locate/jqsrt

# An algorithm for hyperspectral remote sensing of aerosols: 2. Information content analysis for aerosol parameters and principal components of surface spectra

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ARTICLE INFO

*Article history:*
Received 7 October 2016
Received in revised form
1 January 2017
Accepted 3 January 2017
Available online 4 February 2017

*Keywords:*
TEMPO
Geostationary satellite
Information content analysis
Degrees of freedom for signal
Principal component
Hyperspectral remote sensing
Common band selection

ABSTRACT

This paper describes the second part of a series of investigation to develop algorithms for simultaneous retrieval of aerosol parameters and surface reflectance from the future hyperspectral and geostationary satellite sensors such as Tropospheric Emissions: Monitoring of POllution (TEMPO). The information content in these hyperspectral measurements is analyzed for 6 principal components (PCs) of surface spectra and a total of 14 aerosol parameters that describe the columnar aerosol volume $V_{total}$, fine-mode aerosol volume fraction, and the size distribution and wavelength-dependent index of refraction in both coarse and fine mode aerosols. Forward simulations of atmospheric radiative transfer are conducted for 5 surface types (green vegetation, bare soil, rangeland, concrete and mixed surface case) and a wide range of aerosol mixtures. It is shown that the PCs of surface spectra in the atmospheric window channel could be derived from the top-of-the-atmosphere reflectance in the conditions of low aerosol optical depth (AOD $\le$ 0.2 at 550 nm), with a relative error of 1%. With degree freedom for signal analysis and the sequential forward selection method, the common bands for different aerosol mixture types and surface types can be selected for aerosol retrieval. The first 20% of our selected bands accounts for more than 90% of information content for aerosols, and only 4 PCs are needed to reconstruct surface reflectance. However, the information content in these common bands from each TEMPO individual observation is insufficient for the simultaneous retrieval of surface's PC weight coefficients and multiple aerosol parameters (other than $V_{total}$). In contrast, with multiple observations for the same location from TEMPO in multiple consecutive days, 1–3 additional aerosol parameters could be retrieved. Consequently, a self-adjustable aerosol retrieval algorithm to account for surface types, AOD conditions, and multiple-consecutive observations is recommended to derive aerosol parameters and surface reflectance simultaneously from TEMPO.



## 1. Introduction

Atmospheric aerosol properties, especially aerosol optical depth (AOD), have been retrieved routinely from satellite remote sensing since 1990s [1]. While various algorithms have been developed, one of the common and most challenging component in these algorithms is the decoupling of the surface and atmospheric contributions (or path radiance) from the satellite-observed reflectance spectra at the top of atmosphere (TOA), after which aerosol properties can be derived from the path radiance with the correction of Rayleigh scattering and gas absorption [2]. This decoupling is often more complicated over the land than over the ocean for the reason that the contribution of land surface to the radiance measured at the top-of-atmosphere (TOA) is much larger and has various spatial variability in general [3]. Consequently, as shown in Table 1 (for expansion of different satellite acronyms), past algorithms have avoided to conduct retrievals at the spectrum where surface reflectance are high, and instead, focused on the retrieval from use of the spectrum with low land surface reflectance, such as the MODIS visible bands over the vegetated dark target (DT) surfaces [4,5], the MODIS and SeaWiFS "deep blue"

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http://dx.doi.org/10.1016/j.jqsrt.2017.01.041
0022-4073/

**Table 1**
Aerosol parameters have been retrieved from satellite remote sensing.[a]

| Senor | Full name | Parameters retrieved | Assumptions | Spectral used | References |
|---|---|---|---|---|---|
| MERIS | Medium Resolution Imaging Spectrometer | $\alpha$ | $\rho^s$ estimated by linear mixing of different basic spectra with NDVI | 412, 443, 665, 865 nm | [11,12] |
| SCIAMACHY | Scanning Imaging Absorption spectrometer for Atmospheric Chartography | AT | Global $\rho^s$ derived from GOME observation | 364, 387, 429, 683 nm | [10] |
| OMI | Ozone Monitoring Instrument | AT, $\omega$, $H$, PSD | $\rho^s$ from MISR | 15 bands for 330 to 500 nm | [8,9] |
| | | $\tau_a^{388nm}$, $\omega^{388nm}$ | $\rho^s$ from TOMS, dust height from GOCART | 354, 388 nm | [9] |
| SeaWiFS | Sea-Viewing Wide Field-of-View Sensor | $\alpha$ | Global $\rho^s$ dataset, BRDF | 412, 490, 670 nm | [7] |
| MODIS | Moderate Resolution Imaging Spectroradiometer | $\alpha$ | Global $\rho^s$ dataset, BRDF | 412, 470, 650 nm | [6,7] |
| | | $\alpha$, $\eta$ | The empirical relationship of $\rho^s$ at 0.47 (0.66) µm with 2.12µm | 0.47, 0.55, 0.66, 0.86, 1.24, 1.64, 2.12 µm | [4,5] |
| SEVIRI | Spinning Enhanced Visible and Infrared Imager | $r_{\mathrm{eff}}$, AT, $S^{550nm}$ | MODIS BRDF as a priori | 0.64, 0.81, 1.64 µm | [17] |
| AATSR | Advance Along Track Scanning Radiometer | $r_{\mathrm{eff}}$, AT | MODIS BRDF as a priori | 0.55, 0.67, 0.87, 1.6µm, 2 views | [17] |
| MISR | Multi-angle Imaging SpectroRadiometer | AT, MC, SP | BRDF model | 446, 558, 672, 866 nm, 9 views | [13–16] |
| POLDER | Polarization and Directionality of the Earth's Reflectance | $\alpha$ | Log-normal PSD (fine), a priori surface BRDF | 490, 670, 865 nm, up to 16 views and polarization | [19–21] |
| AIRS | Atmospheric Infrared Sounder | $\tau_a^{10\mu m}$ | $r_{\mathrm{eff}}$, Height | 8–12 µm | [22–24] |

[a] The following symbols and acronyms are used in the table as follows. $\tau_a$: AOD, $\rho^s$: surface reflectance, $\eta$: fine mode weighting, $\alpha$: Ångström exponent, $\omega$: single scatter albedo (SSA), $r_{\mathrm{eff}}$: effective radius, $H$: height, $S$: bi-hemispherical albedo, PSD: particle size distribution, AT: aerosol type, MC: mixture of components, SP: (non-) spherical particles.

bands over the urban and semi-arid regions [6,7], and the OMI and SCIAMACHY's ultraviolet (UV) spectrum over ice-free and snow-free land surfaces [8–10]. Besides, some algorithms estimated the surface reflectance by linear mixing of different basic spectra of green vegetation and bare soil with the normalized different vegetation index (NDVI), such as Bremen Aerosol Retrieval (BAER) for MERIS [11,12]. Furthermore, measurements of polarization and/or from multi-angles are shown to make the derivation of path radiance relatively easier, even over the spectrum where surface reflectance is higher. Examples include the empirical orthogonal functions (EOF) algorithm for MISR [13–16], dual-view retrieval algorithm for AATSR [17,18], and polarized retrieval algorithm for POLDER [19–21]. In addition, the thermal infrared (TIR) atmospheric window in 8-12 µm also can be used for characterizing large aerosol particles (such as dust), such as the AIRS's algorithm [22–24]. Table 1 lists the major algorithms for remote sensing of aerosols, including their respective bands, assumptions for deriving surface reflectance, and the aerosol retrieval parameters.

While many progresses were made with past algorithms toward charactering aerosols properties from space, most reliable quantity being retrieved routinely is AOD that is normally characterized at the limited wavelengths or bands. This limitation in part is because that most of these satellite measurements are radiometers with scanning capability in limited number of bands (up to 36 such as MODIS), and in part is restrained by the feasibility to separate the path radiance from surface contributions in various bands (as discussed in the last paragraph). However, a full characterization of aerosol properties requires the retrieval of spectral dependence of aerosol properties (including AOD and absorption), which is also needed in the estimate of radiative forcing of aerosols [25].

This paper presents the second part of a series of studies that aim to develop a hyperspectral remote sensing method for aerosol retrieval from a newly developed GEOstationary Trace gas and Aerosol Sensor Optimization (GEO-TASO) airborne instrument [26]. The GEO-TASO is the airborne version of the upcoming air quality satellite instrument that will measure backscattered ultraviolet (UV), visible (VIS) and near-infrared (NIR) radiation from geostationary orbit, such as Sentinel-4 and Tropospheric Emissions: Monitoring of POllutin (TEMPO) [27,28]. TEMPO was selected as the first Earth Venture Instrument by NASA in 2012 and will be launched between 2019 and 2021 to measure atmospheric pollution for greater North America from space by using hyperspectral UV and visible spectroscopy hourly and with high spatial resolution at $4 \times 4$ km$^2$ [27]. TEMPO will also join Geostationary Environment Monitoring Spectrometer (GEMS) from Korea and Sentianel-4 from Europe as part of the future geostationary satellite constellation [29]. Except for GEO-TASO and TEMPO, other hyperspectral instruments, such as Hyperspectral Infra-Red Imager (HyspIRI), are also under development by NASA [30,31]. Hence, it is necessary to explore and develop algorithms to retrieve aerosols from the hyperspectral measurements.

In the first part of this series of studies, we have developed the theoretical framework of an inversion algorithm to simultaneously retrieve the aerosol properties and surface reflectance. In this framework, it is assumed that surface reflectance spectra can be decomposed into (six) different principal components (PCs) and the wavelength-dependence of aerosol refractive index can be parameterized following a power-law function. These assumptions are generally valid as being supported by the analysis of surface spectra library and Aerosol Robotic Network (AERONET) retrievals [32]. Hence, instead of retrieving surface reflectance at each wavelength, only weight coefficients for each PC are needed to be retrieved.

Based on the framework developed by Hou et al. [32] and the optimal estimation (OE) theory [33], we continue the development of the hyperspectral inversion algorithm by addressing the following feasibility questions: (1) is it possible to obtain the PCs of surface reflectance from the hourly hyperspectral data measured by the instruments (such as TEMPO) in the geostationary (GEO) platform, especially over the surfaces covered by a mixture of different types of canopy? (2) how many and what kind of aerosol parameters can be possibly retrieved together with weighting coefficients for PCs from the hyperspectral data? (3) how can we use GEO's multiple observations with the nearly same Earth-Sun-Satellite geometry in several consecutive days to improve the retrieval? Addressing these questions can provide theoretical guidance in implementing the operational algorithm for aerosol retrieval from GEO-TASO and future geostationary spectrometers.