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Adèle Georgeot, Xavier Ceamanos, Jean-luc Attié. Quantitative assessment of the potential of optimal estimation for aerosol retrieval from geostationary weather satellites in the frame of the iAERUS-GEO algorithm. Atmospheric Science Letters, 2024, 10.1002/asl.1199. hal-04426343

HAL Id: hal-04426343 https://hal.science/hal-04426343

Submitted on 30 Jan2024

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RESEARCH ARTICLE

Quantitative assessment of the potential of optimal estimation for aerosol retrieval from geostationary weather satellites in the frame of the iAERUS-GEO algorithm

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Funding information Météo-France; Région Occitanie Pyrénées-Méditerranée

Abstract

Satellite remote sensing enables the study of atmospheric aerosols at large spatial scales, with geostationary platforms making this possible at sub-daily frequencies. High-temporal-resolution aerosol observations can be made from geostationary data by using robust numerical inversion methods such as the widely-used optimal estimation (OE) theory. This is the case of the instantaneous Aerosol and surfacE Retrieval Using Satellites in GEOstationary orbit (iAERUS-GEO) algorithm, which successfully retrieves aerosol optical depth (AOD) maps from the Meteosat Second Generation weather satellite based on a simple implementation of the OE approach combined with the Levenberg-Marquardt method. However, the exact gain in inversion performances that can be obtained from the multiple and more advanced possibilities offered by OE is not well documented in the current literature. Against this background, this article presents the quantitative assessment of OE for the future improvement of the iAERUS-GEO algorithm. To this end, we use a series of comprehensive experiments based on AOD maps retrieved by iAERUS-GEO using different OE implementations, and ground-based observations used as reference data. First, we assess the varying importance in the inversion process of satellite observations and a priori information according to the content of satellite aerosol information. Second, we quantify the gain of AOD estimation in log space versus linear space in terms of accuracy, AOD distribution and number of successful retrievals. Finally, we evaluate the accuracy improvement of simultaneous AOD and surface reflectance retrieval as a function of the regions covered by the Meteosat Earth's disk.

K E Y W O R D S

aerosols, geostationary satellites, optimal estimation, physical phenomenon, remote sensing, tools and methods

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1 | INTRODUCTION

Aerosols are small particles suspended in the atmosphere coming from natural and anthropogenic sources. Among their various effects, aerosols directly impact the radiative budget of Earth due to their extinction of solar radiation and indirectly contribute to cloud formation and precipitation efficiency (Boucher, 2015). Monitoring aerosols is therefore crucial for weather prediction, climate and solar power, but also for other subjects such as air quality. Aerosols can be measured from different platforms including ground-based stations, aircraft or satellites which, among all observing systems, allow the largest spatial coverage. For example, low Earth orbit (LEO) satellites generally provide one global image per day, whereas geosynchronous equatorial orbit (GEO) satellites acquire multiple images per hour of the Earth disk seen from their position along the geostationary orbit. This high temporal resolution allows GEO satellites to monitor the diurnal variation of aerosols, which can be particularly significant in the instance of mineral dust and air pollutants (Li et al., 2017; Schepanski et al., 2009), but which remain poorly understood nowadays.

Aerosol remote sensing from satellite requires to distinguish the aerosol signature in the signal measured at the top of the atmosphere (TOA), which is also shaped by gases, clouds and surface reflectance. Different quantities linked with aerosols can be retrieved including aerosol optical depth (AOD), which is a proxy for aerosol concentration. Many algorithms exist for aerosol retrieval from satellite data (e.g., Carrer et al., 2014; Ceamanos et al., 2021; Ceamanos et al., 2023; Choi et al., 2016; Dubovik et al., 2021; Govaerts et al., 2010; Govaerts & Luffarelli, 2018; Hsu et al., 2013; Jeong et al., 2016; Katsev et al., 2010; Kim et al., 2018; Levy et al., 2013; Sayer et al., 2016; Thomas et al., 2009; Vandenbussche et al., 2020; Waguet et al., 2016; Yoshida et al., 2018), some of them using look-up tables of pre-calculated TOA measurements and some others using a radiative transfer model (RTM) coupled with a numerical inversion method. In the latter case, we find for example the optimal estimation (OE) theory based on Bayes' theorem which is being increasingly used in recent times (Rodgers, 2000). Since aerosol retrieval is a non-linear problem, least-squares minimization methods like Newton, Gauss-Newton and Levenberg-Marquardt (LM) are well indicated to solve it.

Some of the satellite aerosol retrieval algorithms cited above use the LM method in the frame of OE, as it is described in Rodgers (2000). This is the case of the instantaneous Aerosol and surfacE Retrieval Using Satellites in GEOstationary orbit (iAERUS-GEO) algorithm (Ceamanos et al., 2023) for which a simple version of the

LM method was implemented to retrieve AOD in view of several features of interest including the possibility of using a priori information. Prior data can help to ease the calculation of retrievals from satellite observations with low information content on aerosols. This becomes particularly interesting in the case of GEO satellites as it contributes to achieve a continuous, high-frequency flow of accurate aerosol retrievals. The current version of iAERUS-GEO does not exploit other more advanced LM features such as the retrieval of multiple variables simultaneously. While these possibilities may be useful for the future evolution of this algorithm, the exact gain in inversion accuracy and in the number of successful retrievals that can be obtained from their implementation is not well documented in the current literature, particularly in the case of GEO remote sensing.

In this context, this article proposes a quantitative assessment of the benefits of several possibilities offered by OE in the framework of the future improvement of iAERUS-GEO. This is achieved by conducting a series of comprehensive experiments with different implementations of the OE-LM approach using data from the Spinning Enhanced Visible and InfraRed Imager (SEVIRI) on the GEO weather satellite Meteosat Second Generation (MSG), as well as ground-based AOD measurements used for validation. First, we assess the benefits of the LM method, and in particular of the use of a priori information, to estimate AOD as it is currently implemented in iAERUS-GEO. Second, the improvement in inversion performances from more advanced possibilities of the LM method are evaluated quantitatively, including the simultaneous estimation of AOD and surface reflectance but also the inversion of AOD in log space. Finally, and based on the obtained results, we draw conclusions on the benefits that using OE may have on the evolution of iAERUS-GEO for aerosol retrieval from the new GEO mission Meteosat Third Generation-Imager (MTG-I).

2 | METHODS

2.1 | Aerosol retrieval algorithm: iAERUS-GEO

iAERUS-GEO (Ceamanos et al., 2023) is a complex algorithm that provides maps of AOD over land and ocean for diurnal cloud-free conditions. It was initially developed to process data from the SEVIRI multi-spectral imager onboard the MSG satellite from the European Organisation for the Exploitation of Meteorological Satellites (EUMETSAT). SEVIRI is a scanning radiometer with 12 spectral channels, ranging from the visible to the infrared spectral ranges, and a maximum spatial resolution of 3 km at the sub-satellite point. AOD is estimated by iAERUS-GEO every 15 min (i.e., the acquisition frequency of SEVIRI) at 0.635 µm, which corresponds to the central wavelength of the shortest SEVIRI channel named VIS06. The algorithm uses seven realistic aerosol models defined by optical properties that are representative of the AErosol RObotic NETwork (AERONET) regional climatology in different parts of the world (i.e., desert dust, maritime, biomass burning, continental Europe, continental USA, arid and polluted India) and takes different inputs including TOA radiance, solar and viewing angles, cloud/snow mask and data on atmospheric composition. Three main processing steps can be identified:

- · Rayleigh scattering and gas absorption are corrected using atmospheric fields of total column ozone, total column water vapour and surface pressure. Only best-quality SEVIRI observations (unaffected by clouds, snow, sun glint or very high zenith angles) are used here.
- AOD is retrieved for each SEVIRI image, at the satellite's native spatial resolution, with the LM method coupled to an efficient RTM. A dynamic (varying with time and space) AOD climatology is used as a priori information (Section 3.2.1). Spatio-temporal multipixels are used to retrieve AOD to impose the natural smoothness of aerosols with time and space.
- Surface reflectance, which is required to estimate AOD due to the strong aerosol-surface coupling in the visible domain, is obtained by estimating the bidirectional reflectance distribution function (BRDF) also at 0.635 µm at the end of each day using a recursive Kalman filter-based method. The main assumption of this step is that land surface properties are more stable in time compared to AOD.

iAERUS-GEO was successfully validated with AERO-NET ground-based data, with an average root-meansquare error (RMSE) of 0.115, a mean bias error (MBE) of 0.024, a mean correlation factor (R) of 0.769 and more than 50 times retrievals compared to AOD products based on LEO satellites. This accuracy proved comparable to that of state-of-the-art aerosol retrieval algorithms, as detailed in Ceamanos et al. (2023).

Implementation of the LM method 2.2

2.2.1 | AOD estimation

Here we present the LM method and explain how it is currently implemented in the current iAERUS-GEO algorithm (Ceamanos et al., 2023).

At each iteration *i* of the method, the estimated variable *x* is updated with the formula:

$$\begin{aligned} x_{i+1} &= x_a + \left(K_i^T S_{\varepsilon}^{-1} K_i + (1+\gamma) S_a^{-1} \right)^{-1} \\ & \left(K_i^T S_{\varepsilon}^{-1} ((\rho_{obs} - \rho_{sim}(x_i)) + K_i(x_i - x_a)) \right) \\ & + \gamma S_a^{-1}(x_i - x_a) \right), \end{aligned}$$
(1)

where x_a is the a priori value, K_i the Jacobian of x_i , S_{ϵ} the observation error covariance matrix quantifying the error from the satellite data, γ a damping factor and S_a the a priori covariance matrix. S_a is used to control how far x_i departs from x_a , and S_{ε} is used to control how far the satellite signal estimated with x_i departs from the satellite observation. ρ_{obs} is the observed satellite reflectance and ρ_{sim} is the simulated reflectance calculated by the RTM included in iAERUS-GEO. Covariance matrices are determined based on available information on the SEVIRI sensor uncertainty and the natural distribution of AOD (see Section 3.1 for more details).

At each iteration, the cost function χ^2 is updated by doing:

$$\chi_{i+1}^{2} = (x_{i+1} - x_{a})^{T} S_{a}^{-1} (x_{i+1} - x_{a}) + (\rho_{obs} - \rho_{sim}(x_{i+1}))^{T} S_{\varepsilon}^{-1} (\rho_{obs} - \rho_{sim}(x_{i+1})).$$
(2)

Two cases are then considered after comparing χ^2_{i+1} to χ_i^2 (with γ set initially to 1):

- If $\chi_{i+1}^2 < \chi_i^2$, γ is divided by α (which is set to 2). Then, x_{i+2} is calculated.
- If $\chi_{i+1}^2 > \chi_i^2$, γ is multiplied by α , and a new loop begins until $\chi_{i+1}^2 < \chi_i^2$ or until the maximum number of iterations of that loop is reached. Then, x_{i+2} is calculated.

The retrieval stops when the maximum number of iterations of the first loop is reached. Currently in iAERUS-GEO, only AOD is estimated.

AOD estimation in the log space 2.2.2

Optimal estimation assumes that the estimated variables follow a normal distribution. However, this hypothesis is not valid for AOD, which is known to follow a log-normal distribution (O'Neill et al., 2000). Furthermore, the inversion method previously presented in Section 2.2.1 allows negative retrievals, which are not physically possible for AOD. To avoid

these issues, we perform the estimation of AOD in the log space as done in Dubovik et al. (2021) to (1) force the retrievals to be positive and (2) transform the lognormal law that is naturally followed by AOD into a normal law. The latter point aims at making the AOD distribution more consistent with the optimal estimation theory.

The retrieval is achieved in the log space by modifying Equation (1) into

$$\begin{aligned} \log(x_{i+1}) &= \log(x_{a}) + \left(\log(K_{i})^{T} S_{\varepsilon-\log}^{-1} \log(K_{i}) + (1+\gamma) S_{a-\log}^{-1}\right)^{-1} \\ & \left(\log(K_{i})^{T} S_{\varepsilon-\log}^{-1} \left((\log(\rho_{obs}) - \log(\rho_{sim}(x_{i}))) + \log(K_{i}) (\log(x_{i}) - \log(x_{a})) \right) + \gamma S_{a-\log}^{-1} (\log(x_{i}) - \log(x_{a})) \right) \end{aligned}$$

$$(3)$$

and Equation (2) into

$$\begin{split} \chi^{2}_{i+1} &= (\log(x_{i+1}) - \log(x_{a}))^{T} S^{-1}_{a-log} (\log(x_{i+1}) - \log(x_{a})) \\ &+ (\log(\rho_{obs}) - \log(\rho_{sim}(x_{i+1})))^{T} S^{-1}_{\varepsilon-log} (\log(\rho_{obs}) - \log(\rho_{sim}(x_{i+1}))). \end{split}$$

$$(4)$$

We applied the logarithm to all variables, except for $S_{\varepsilon-log}$ and S_{a-log} that are determined based on available information as in the case without log. The Jacobian is calculated as $\log(K_i) = \frac{K_i}{\rho_{sim}(x_i)}$. Again, only AOD is retrieved here.

2.2.3 | Simultaneous estimation of AOD and surface reflectance in the log space

Here we improve the LM method implementation presented in Section 2.2.2 to retrieve surface reflectance in addition to AOD. This is done to correct potential biases in the surface BRDF retrieved in the third step of iAERUS-GEO (Section 2.1) and that can heavily impact AOD retrieval in the case of strong aerosol-surface coupling. In practice, surface reflectance is refined with respect to the estimate provided by iAERUS-GEO by using this information as prior data and by choosing a low value for the prior covariance matrix element corresponding to surface reflectance. Equations (3) and (4) are used in this configuration. In this case, the retrieved quantity is a vector of size 2 ($x_i = (\tau_i, \rho_s)$), (τ_i representing the estimated AOD, and ρ_s surface reflectance) as well as the Jacobian K_i , and S_a is a 2 × 2 matrix assuming that AOD and surface reflectance are independent (Yoshida et al., 2018).

3 | EXPERIMENTAL PROTOCOL AND DATA

3.1 | Test design

The experiments conducted in this research are detailed as follows (see Table 1 for more details including the covariance matrices):

- Experiment 0: Current version of iAERUS-GEO (Ceamanos et al., 2023).
 - Exp. 0: using the LM inversion method described in Section 2.2.1 with the dynamic AOD climatology (Section 3.2.1) as prior. We determined S_a as the variance of the normal distribution that yielded the best fit of the histogram of the AERONET AOD data used in this study, with the mean of the normal distribution equal to the average value of the AERO-NET AOD data. The value of S_e was defined to encompass the uncertainty of the SEVIRI VIS06 channel (equal to 3% according to Luffarelli & Govaerts, 2019) and other errors operating in the inversion process such as those originating from the forward RTM.
- Experiment 1: importance of prior information.
 - Exp. 1a: same as Exp. 0 without any a priori constraint, which is achieved by setting a very high value for the a priori AOD variance S_a .
 - Exp. 1b: same as Exp. 0 but using a static a priori information, which is set to the mean value of the dynamic AOD climatology (i.e., AOD = 0.18; see Figure 1c) to allow a fair comparison with Exp. 0 in terms of the bias affecting prior data.
 - Exp. 1c: iAERUS-GEO is not run here and retrievals are simply set to the a priori values coming from the dynamic AOD climatology used in Exp. 0. This experiment aims to investigate the independence of retrievals from Exp. 0 on prior data.
- Experiment 2: further improvements with LM.
 - Exp. 2a: same as Exp. 0 but using the LM method in the log space (Section 2.2.2). S_{a-log} was determined similarly as S_a in Exp. 0, by determining the variance yielding the normal distribution that fits the best the histogram of the logarithm of the AERO-NET AOD data.
 - Exp. 2b: same as Exp. 0 but simultaneously estimating AOD and surface reflectance in the log space (Section 2.2.3). The AOD variance is equal to that of Exp. 2a. The surface reflectance variance was determined by fitting the histogram of surface reflectance initially estimated by iAERUS-GEO

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TABLE 1 List of experiments with their setup. Max-iter1 and Max-iter2 were determined empirically.

Experiment	Description	Retrieved variables	Sa	$oldsymbol{S}_arepsilon$	Max-iter1	Max-iter2
Exp. 0	Dynamic prior	AOD	0.05	0.0001	8	8
Exp. 1a	No prior	AOD	5	0.0001	8	8
Exp. 1b	Static prior	AOD	0.05	0.0001	8	8
Exp. 1c	Climatology	AOD	-	-	-	-
Exp. 2a	Logarithm	AOD	0.9	0.006	25	3
Exp. 2b	ρ_s refinement	AOD, ρ_s	$\begin{pmatrix} 0.9 & 0 \\ 0 & 0.0003 \end{pmatrix}$	0.006	25	3

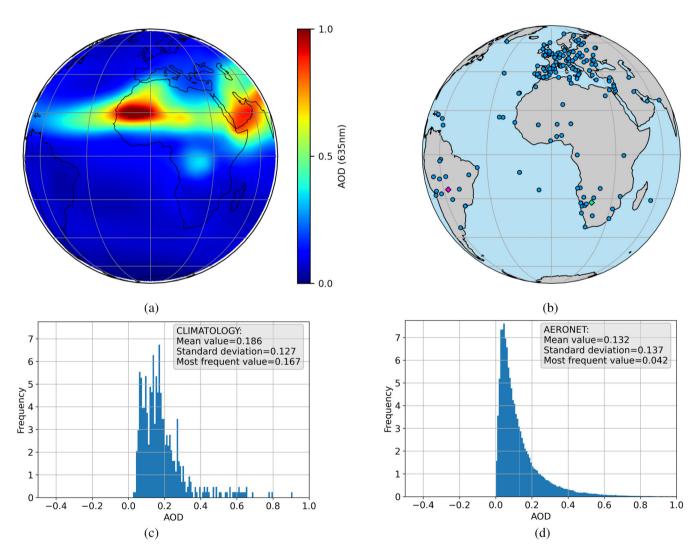


FIGURE 1 (a) Dynamic AOD climatology used as prior data for July. (b) Location of the AERONET stations considered in this study, with *CUIABA-MIRANDA* and *Bonanza* sites highlighted with a magenta and green rhombus, respectively. (c) Histogram of the dynamic AOD climatology limited to the location of the AERONET stations and the period of study, from June to August 2016. (d) Histogram of the AOD retrieved from sun photometers at the AERONET stations for the period of study.

(Section 2.1). However, a smaller value than the best-fit variance was chosen to impose a higher weight on the prior surface reflectance, which is

assumed to be reliable overall based on the satisfactory results when surface reflectance is not refined (e.g., Exp. 2a). All experiments were conducted by processing the SEVIRI data corresponding to the location of the AERONET sites falling into the MSG Earth's disk (see Figure 1b). The period of summer 2016 (June, July and August) was considered.

3.2 | Input data

We used SEVIRI observations corresponding to the period and locations of interest as input for all experiments. ERA5 reanalyses from the European Centre for Medium-Range Weather Forecasts (Hersbach et al., 2020) were used for the required atmospheric fields (see Section 2.1) and the NWC-SAF (Satellite Application Facility on Support to Nowcasting and Very Short Range Forecasting) software was used to generate the required cloud masks (Derrien & Le Gleau, 2005).

3.2.1 | Dynamic AOD prior information

The current version of iAERUS-GEO (Exp. 0) uses monthly means of AOD across the SEVIRI disk as prior information. This dynamic data set, both in time and space, was constructed based on the aerosol climatology from the Copernicus Atmosphere Monitoring Service (Bozzo et al., 2020). The map of prior AOD used in July is shown in Figure 1a. The distribution of the prior AOD values corresponding to the 3 months of the period of study is shown in Figure 1c.

3.3 | Evaluation data

We used AOD retrievals from ground stations (Figure 1b) belonging to the AERONET network of sun photometers (Holben et al., 1998) to evaluate the satellite retrievals obtained in this study. AOD values from AERONET (version 3 algorithm, quality level 2.0, Giles et al., 2019) were resampled to match the 15-min frequency of SEVIRI and converted to 635 nm with the corresponding Ångström exponent. The histogram in Figure 1d shows the distribution of the AERONET data used in this study.

4 | RESULTS

4.1 | Experiment 0: Current version of iAERUS-GEO

Figure 2a presents the assessment of iAERUS-GEO retrievals with respect to AERONET, with average scores

of 0.112 for RMSE, 0.027 for MBE and 0.767 for *R*. These scores are very similar to the ones obtained in Ceamanos et al. (2023). The mean AOD value is moderately overestimated (0.17, as opposed to 0.14 for AERONET), which can be explained by the higher mean value of the dynamic AOD climatology used as prior with respect to AERONET data (0.186 vs. 0.132; see Figure 1c,d). There is a high number of retrievals in total (151,291) corresponding to a mean of 11 estimations per day and per site.

4.2 | Experiment 1: Importance of a priori information

First, Figure 2b shows that the retrieved AOD becomes less accurate when a priori information is not considered (Exp. 1a). The scores are degraded with regard to Exp. 0, with RMSE increasing from 0.112 to 0.137, MBE increasing from 0.027 to 0.039 and R decreasing from 0.767 to 0.669. Moreover, we obtain less retrievals (136,979 vs. 151,291) due to the higher number of negative AOD retrievals that are obtained when no prior data are used (n.b., only positive retrievals are considered in the comparison with AERONET).

Second, Figure 2c shows that the use of a static prior (Exp. 1b) has a negative impact on the retrieved AOD with respect to the experiment with a dynamic prior (Exp. 0). RMSE and MBE are quite similar, whereas R significantly decreases from 0.767 to 0.699.

Finally, we observe in Figure 2d that the AOD dynamic climatology used as prior by the current version of iAERUS-GEO shows some bias with respect to AERO-NET data in our case study. This is reflected in the decrease in correlation from 0.767 to 0.517, the increase in MBE from 0.027 to 0.072 and the increase in RMSE from 0.112 to 0.144.

Results are summarized in Table 2.

4.3 | Experiment 2: Going further with LM

4.3.1 | AOD retrieval in the log space

Table 2 and Figure 2e show that the inversion in the log space (Exp. 2a) improves all the average scores obtained by the retrieved AOD values with respect to Exp. 0. RMSE decreases from 0.112 to 0.108, MBE decreases from 0.27 to 0.19 and *R* increases from 0.767 to 0.778. Furthermore, we observe a significant increase in the

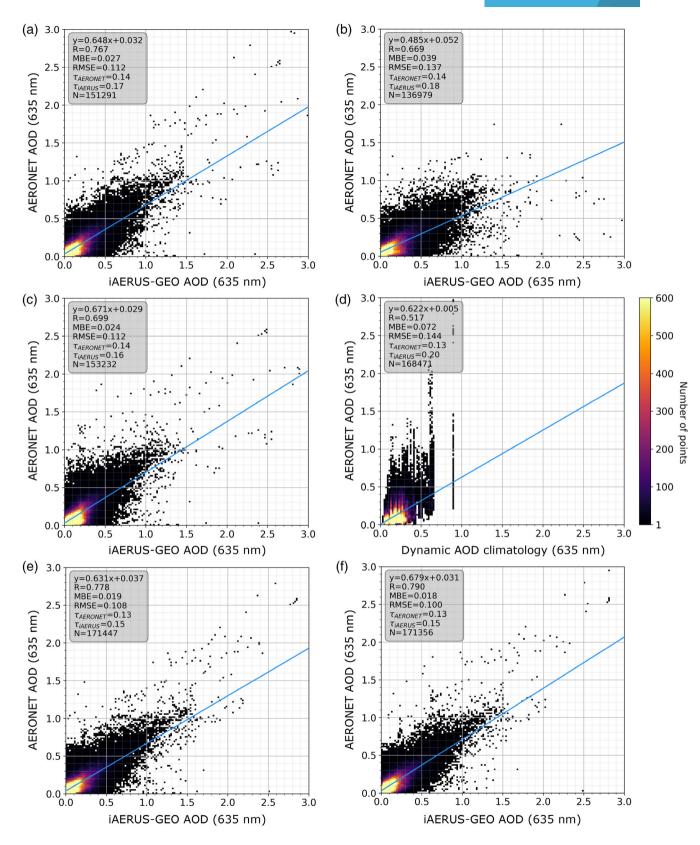


FIGURE 2 Density scatter plots comparing AOD retrieved by AERONET and iAERUS-GEO in the configurations with (a) the current algorithm version (Exp. 0), (b) no prior (Exp. 1a), (c) a static prior (Exp. 1b), (d) the dynamic AOD climatology as output (Exp. 1c), (e) inversion in log space (Exp. 2a), and (f) surface reflectance refinement (Exp. 2b).

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Experiment	RMSE	Bias	R	N	Mean AOD
Exp. 0—dynamic prior	0.112	0.027	0.767	151,291	0.17
Exp. 1a—no prior	0.137	0.039	0.669	136,979	0.18
Exp. 1b—static prior	0.112	0.024	0.699	153,232	0.16
Exp. 1c—climatology	0.144	0.072	0.517	168,471	0.18
Exp. 2a—logarithm	0.108	0.019	0.778	171,447	0.15
Exp. 2b— ρ_s refinement	0.100	0.018	0.790	171,356	0.15

TABLE 2 Scores obtained for the different retrieval experiments with respect to AERONET: root mean square error (RMSE), mean bias error (MBE), correlation coefficient (*R*), number of retrievals (*N*), and mean value of the retrieved AOD.

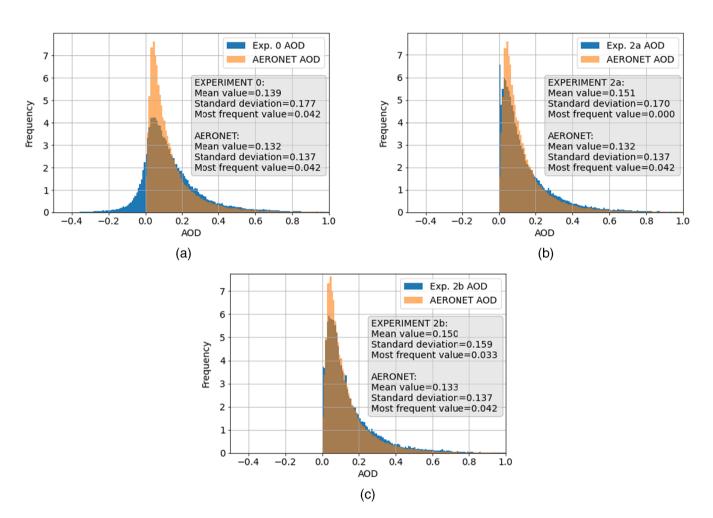


FIGURE 3 Comparison of AOD histograms from AERONET and iAERUS-GEO for (a) Exp. 0 with dynamic prior, (b) Exp. 2a with dynamic prior and log space, and (c) Exp. 2b with dynamic prior, log space, and surface reflectance refinement.

number of retrievals, from 151,291 to 171,447 successful estimations (+13%).

Figure 3 confirms the improvement achieved with Exp. 2a by comparing the histograms of the AOD retrieved from satellite to AERONET. We observe that the histogram of Exp. 0 shows some significant differences with regard to the AERONET histogram, with especially recurrent negative AOD values (Figure 3a). Most of these dissimilarities disappear when the inversion is made in the log space (Figure 3b).

4.3.2 | AOD and surface reflectance retrieval

Figure 3c shows the added value of the simultaneous retrieval of AOD and surface reflectance (Exp. 2b), with the further increase of similarity between iAERUS-GEO and AERONET histograms. Overall, the scores obtained with Exp. 2b are improved compared to Exp. 2a, with RMSE decreasing from 0.108 to 0.100, MBE decreasing from 0.019 to 0.018, and *R* increasing from 0.778 to 0.790 (Table 2; Figure 2f).

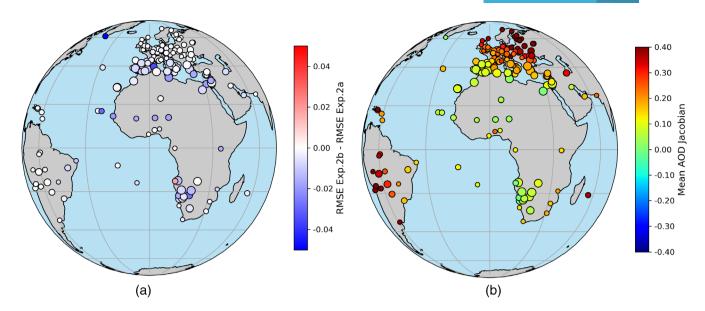


FIGURE 4 (a) Difference of average RMSE between Exp. 2b and Exp. 2a and (b) mean AOD Jacobian for Exp. 2b over the period of study for all AERONET stations. The size of dots is proportional to the number of AOD retrievals.

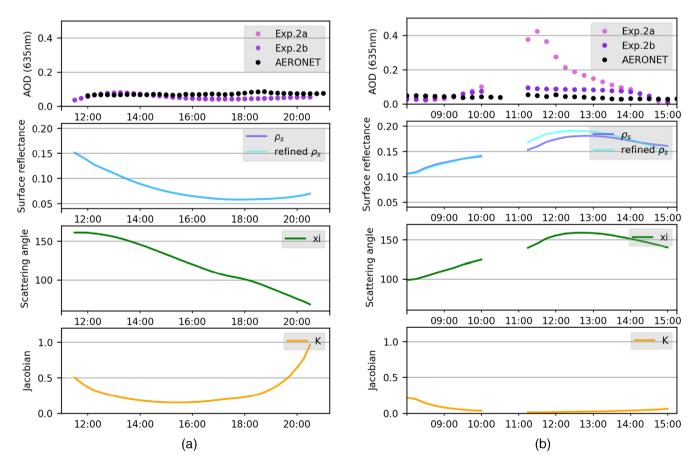


FIGURE 5 Zooming in on the inversion performed by iAERUS-GEO in Exp. 2a and Exp. 2b in terms of, from top panel to bottom panel, AOD, surface reflectance, scattering angle, and AOD Jacobian (calculated for Exp. 2b) for (a) *CUIABA-MIRANDA* site on 18 July 2016 and (b) *Bonanza* site on 24 June 2016.

Figure 4a confirms the benefits of this multi-parameter retrieval by showing that the average RMSE is improved from Exp. 2a to Exp. 2b, especially in southern Europe and Africa. Figure 4b shows mean values of AOD Jacobian (calculated for Exp. 2b) close to 0 in these regions, which means that the AOD sensitivity from

SEVIRI observations is low in this case. This low information content is due to a combination of factors including lower aerosol scattering and brighter surface reflectance, usually happening at higher scattering angles (Ceamanos et al., 2019). Figure 4 shows that refining the surface reflectance initially estimated by iAERUS-GEO improves AOD retrievals, especially when the sensitivity to aerosols is low. This was confirmed by additional experiments that showed a greater improvement of AOD retrievals thanks to surface reflectance refinement in the case of low Jacobian values (see Table S1 in the Supporting Information).

Figure 5 confirms that surface reflectance refinement mostly impacts AERONET stations with low sensitivity to AOD. For the CUIABA-MIRANDA site in Brazil (see magenta rhombus in Figure 1b), which is located in a region with high information content (Figure 4b), there is almost no difference in the retrieved AOD values mainly due to the generally high AOD Jacobian and low scattering angle (Figure 5a). However, for the Bonanza site in Namibia (see green rhombus in Figure 1b), AOD is initially overestimated due to an AOD Jacobian close to 0 during most of the day (Figure 5b). This bias is greatly overcome with the refinement of the surface reflectance, which is noticeably increased in Exp. 2b (second panel of Figure 5b). By contrast, we can see that surface reflectance is not modified in the case of the CUIABA-MIRANDA site.

5 | CONCLUSIONS

Although OE has been used for a number of years for satellite aerosol retrieval, the exact gain in inversion performance to be expected from its multiple possibilities is not well documented in the current literature. This is particularly true in the case of great-temporal-revisit GEO satellites, where the interest is not only in the potential increase in inversion accuracy, but also in the number of successful inversions. Here, we assess and quantify the value added by several features of OE, combined with the LM method, in the frame of the iAERUS-GEO algorithm retrieving AOD from GEO data. This is done by a series of comprehensive experiments using satellite observations from the MSG/SEVIRI weather mission and ground-based measurements from the AERONET network. First, we assess in Experiment 1 the gain in AOD accuracy and number of retrievals obtained from a good balance between the satellite observations and a priori information. On the one hand, the use of prior information helps to retrieve 10% more of AOD values that make sense physically, with regard to the case not using a priori. The additional inversions mainly correspond to

challenging situations where information content on aerosols is low. The benefits of using prior data are particularly significant when a dynamic climatology is selected as prior instead of a constant value, with a correlation increasing from 0.699 to 0.767. On the other hand, satellite observations are proved to be the main source of information in most situations, making retrievals independent from a priori information. This is seen by the drop of correlation from 0.767 to 0.517 if the AOD from the dynamic climatology used in the current implementation of iAERUS-GEO is compared to AERONET. Second, Experiment 2 shows that further improvements are possible for the future evolution of iAERUS-GEO thanks to the additional features of the LM method. The first advance is achieved with the retrieval of AOD in the log space, which provides not only more estimations (+13%)with respect to the inversion in the linear space but also more accurate retrievals (e.g., bias decrease of 29%), and an AOD distribution closer to the log-normal distribution naturally followed by aerosols. The second improvement that was assessed is the simultaneous retrieval of AOD and surface reflectance, which allows the reduction of AOD errors (-7% for both RMSE and MBE) in regions where satellite sensitivity to aerosols is low.

The results obtained in this study provide relevant information for the future evolution of the iAERUS-GEO algorithm and, in particular, for its adaptation to the new Flexible Combined Imager (FCI)/MTG-I weather mission launched in December 2022. FCI will provide Earth images from the GEO orbit with additional spectral channels in the visible and near infrared ranges compared to SEVIRI, including a channel sensing the blue wavelength that is of particular interest for aerosol retrieval (Aoun, 2016; Hsu et al., 2013). The simultaneous processing of these new channels, and others already existing on SEVIRI, for inversion may offer new possibilities in aerosol characterization, including the improved estimation of AOD but also the retrieval of additional parameters related to the nature of particles, as well as land surface properties such as albedo (Juncu et al., 2022). In this context, the advanced features of OE that have been evaluated in this paper, mainly the possibility of estimating several variables simultaneously, may become great interest in the future evolution of iAERUS-GEO.

AUTHOR CONTRIBUTIONS

Adèle Georgeot: Data curation; formal analysis; investigation; methodology; validation; visualization; writing – original draft. **Xavier Ceamanos:** Conceptualization; data curation; funding acquisition; investigation; methodology; project administration; supervision; validation; visualization; writing – review and editing. Jean-Luc Attié: Conceptualization; formal analysis;

Atmospheric Science Letters

funding acquisition; methodology; supervision; validation; writing – review and editing.

ACKNOWLEDGMENTS

We would like to thank the investigators and their staff for establishing and maintaining the AERONET sites used in this work. We thank the AERIS/ICARE Data and Services Center for providing the input data used in this study. Adèle Georgeot would like to thank Rémy Fransen for his help with data processing. We finally thank the three anonymous reviewers for their comments on the manuscript.

FUNDING INFORMATION

This research has been partly supported by the Région Occitanie Pyrénées-Méditerranée and Météo-France.

CONFLICT OF INTEREST STATEMENT

The authors declare no conflicts of interest to disclose.

DATA AVAILABILITY STATEMENT

The data used in this article are available upon request from the corresponding author.

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SUPPORTING INFORMATION

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How to cite this article: Georgeot, A., Ceamanos, X., & Attié, J.-L. (2023). Quantitative assessment of the potential of optimal estimation for aerosol retrieval from geostationary weather satellites in the frame of the iAERUS-GEO algorithm. *Atmospheric Science Letters*, e1199. <u>https://doi.org/</u>10.1002/asl.1199