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A Generalized Aerosol Algorithm for Multi-Spectral Satellite Measurement With Physics-Informed Deep Learning Method

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Key Points:

- A generalized aerosol algorithm is developed based on physics-informed deep learning (PDL) method for multi-spectral satellite measurement
- MODIS PDL retrieval has not only high accuracy in AOD and fine AOD, but also marked sensitivity to coarse AOD and aerosol absorption
- PDL method can make full use of the multi-spectral satellite measurement and prior information with high computational efficiency

Supporting Information:

Supporting Information may be found in the online version of this article.

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Abstract

The multi-spectral satellite sensors such as MODIS have a large swath, high spatial resolution, and well onboard calibration, enabling aerosol retrievals with daily global coverage. Despite numerous available bands, MODIS aerosol algorithms over land typically only utilize measurements from 2 to 3 spectral wavelengths to retrieve Aerosol Optical Depth (AOD) based on prescribed aerosol models. To make full use of multi-spectral measurements and prior information, we developed an aerosol algorithm based on physics-informed deep learning (PDL) approach. With physical constraint from radiative transfer simulation, PDL can construct model functions between the whole spectral measurements and each retrieved aerosol parameter separately. AERONET validations in eastern China show that MODIS PDL algorithm can accurately retrieve AOD and fine AOD ($R = 0.936$) at 1 km resolution and has reliable performance in coarse AOD as well as notable sensitivity to aerosol absorption. The flexible and efficient PDL method provides a generalized algorithm for common multi-spectral satellite measurements.

Plain Language Summary

Atmospheric aerosols play a crucial role in the Earth's radiative energy balance, hydrological cycle, and air quality as well as biogeochemical cycles. Owing to short lifetime and diverse emission sources, aerosol amount and properties vary largely over space and time, making a great challenge in quantifying its climate and environmental effects. With the recognition of aerosols' important role, dedicated satellite instruments have been launched to obtain global aerosol observations since late 1990s. Despite a lack of angular and polarized information, current widely used satellite aerosol products are mainly derived from multi-spectral measurement due to their daily global coverage and long-term well-calibrated observation. However, common algorithms only utilize 2–3 spectral measurements and retrieve one quantitative Aerosol Optical Depth with prescribed aerosol models. By combining the physical constraints from Radiative Transfer simulation and modeling ability of Deep Learning, we developed a generalized physics-informed DL method that can make full use of multi-spectral measurements and prior information for aerosol retrievals.

1. Introduction

Atmospheric aerosols play a crucial role in governing the Earth's radiative energy balance, affecting hydrological cycle, air quality, and biogeochemical cycles (Kaufman et al., 2002). Their lifetimes span a few hours to several days and their emissions are from diverse sources at various spatial scales. As such, the distribution of aerosol amount and properties vary significantly over space and time, making it a great challenge to quantify their climate and environmental effects. Therefore, accurate and continuous observation of aerosol properties from regional to global scales is a critical requirement in climate and air quality studies.

Over the past decades, dedicated satellite instruments such as the Moderate Resolution Imaging Spectroradiometer (MODIS), Multi-angle Imaging SpectroRadiometer (MISR), and POLarization and Directionality of the Earth's Reflectances (POLDER) have been launched to collect global aerosol observations (King et al., 1999). Those observations have greatly advanced our knowledge concerning global aerosol hotspots and main emitting sources (Chen et al., 2020; Kahn & Gaitley, 2015; Levy et al., 2013). Sophisticated MISR and POLDER measure radiance (and polarization from POLDER) from multi-view angles and thus yielding more information regarding aerosol microphysical properties, but their swath width or pixel resolution is limited compared with multi-spectral

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instruments such as MODIS. Though as the only one quantitative aerosol parameter, MODIS Aerosol Optical Depth (AOD) has been the most widely used satellite aerosol parameter due to its near-daily global coverage.

Since there are too many aerosol and surface's unknowns, standard MODIS aerosol retrieval algorithms typically utilize pre-defined aerosol models in look-up tables (LUT) and pre-calculated reflectance or their empirical relationships (Hsu et al., 2013; Levy et al., 2013; Lyapustin et al., 2018). By using satellite measurements at 2–3 spectral bands typically, these LUT-based algorithms retrieve AOD and fine mode fraction, which have considerable bias with only one quantitative AOD (Tao et al., 2019). Recently, algorithms using Deep Learning (DL) methods have emerged and been shown to offer aerosol retrievals with a higher accuracy than the traditional LUT algorithms in regional scales. Those DL-based algorithms build upon direct relationship between observed satellite reflectance at the top of the atmosphere (TOA) and AOD and fine mode AOD (FAOD) as observed by Aerosol Robotic Network (AERONET) or the relationship between simulated TOA reflectance and AOD at more spectral wavelengths (Jia et al., 2022; Kang et al., 2022). Despite the powerful modeling ability of DL methods, it still lacks a clear and unified physical basis regarding to how to make full use of various multi-spectral satellite measurements for aerosol retrievals.

In this study, we developed a generalized algorithm for retrieving multiple aerosol parameters from multi-spectral satellite measurements based on a physics-informed DL (PDL) method. Section 2 introduces the MODIS and AERONET data, which are used to demonstrate the performance of the algorithm. The principle of the PDL algorithm suited for aerosol retrievals from MODIS observations is described in Section 3. Then we evaluate our PDL-based retrievals by validation against AERONET measurements and by inter-comparisons with standard MODIS aerosol products. Section 5 summarizes our main findings and conclusions.

2. Data and Methods

2.1. MODIS Aerosol Products

Since 2000 and 2002 respectively, MODIS instruments onboard the Terra and Aqua satellites have been measuring radiances of the Earth-atmosphere system in 36 spectral bands from 0.4 to 14 μm along with dedicated on-orbit calibrations. With a wide swath of ∼2,330 km, MODIS measurements achieve a near-daily global coverage at a pixel resolution of 250–1,000 m at nadir. There have been several operational MODIS aerosol products from Dark Target (DT), Deep Blue (DB), and Multi-Angle Implementation of Atmospheric Correction (MAIAC) algorithms (Hsu et al., 2013; Levy et al., 2013; Lyapustin et al., 2018). Those algorithms make use of lookup table (LUT) methods involve pre-calculated relationship between MODIS observations and aerosol parameters for various aerosols models. Moreover, their retrievals estimate surface reflectance from their linear relationship at visible and shortwave infrared bands or minimal ratio, and pre-calculated database, respectively. Here we select Collection (C) 6.1 MODIS DB at 10 km and C6 MAIAC AOD at 1 km for inter-comparison with our retrievals (Tao et al., 2019).

2.2. AERONET Data

AERONET is a global remote sensing network of Sun photometers that provides spectral AOD and inversions of aerosol microphysical parameters (Giles et al., 2019). Derived from direct sunlight, AERONET AODs have a very high accuracy of ∼0.01–0.02. By combining spectral AODs with directional sky light, aerosol microphysical parameters including spectral complex refractive index, size distribution at 22 bins, and fraction of non-spherical particles are retrieved in AERONET inversions (Dubovik et al., 2002; Sinyuk et al., 2020). We select AERONET Level 2.0 or Level 1.5 data at 13 sites in eastern China for validation (Figure S1 in Supporting Information S1). For matchup of satellite and ground data, a spatial window of 25 km radius for MODIS pixels and a time window of ±30 min for AERONET AOD and SSA are used, respectively.

3. Multi-Spectral Satellite Aerosol Retrieval With Physics-Based DL (PDL) Method

To retrieve aerosol properties from satellite measurements, a basic premise is to establish an accurate forward radiative transfer (RT) model that gives physical equations to solve aerosol/surface unknowns. Reliable RT simulations provide a unique and physical function between parameters of aerosol and surface and satellite measurements in each calculation, which can be used to generate training samplings for DL aerosol retrievals. Then, DL

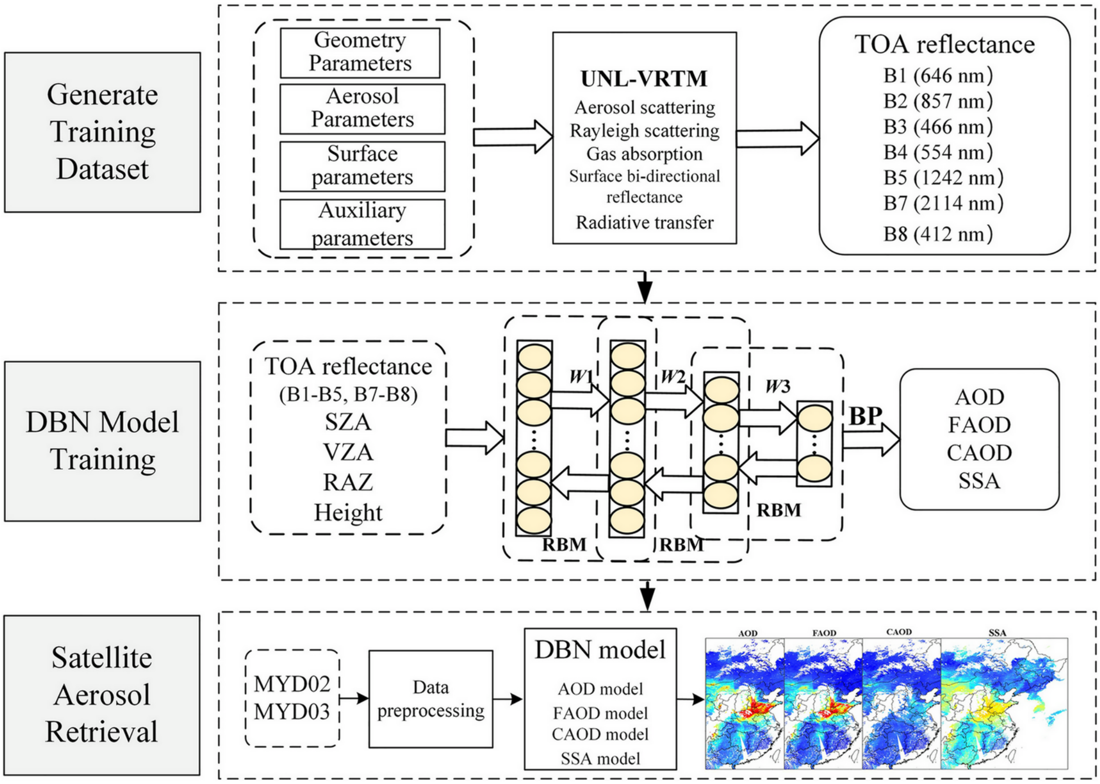

Figure 1. The flowchart of PDL aerosol algorithm for MODIS measurements.

methods can be used to derive the high-order relationships between simulated satellite observations and aerosol parameters. In the optimized inversions, iterative RT calculations of all aerosol/surface unknowns can propagate uncertainties of unknowns with low information content to the whole retrieval. With the physical constraint from RT simulations, PDL method can directly build the model function between satellite spectral TOA reflectance and each interested aerosol parameter separately and flexibly. The accuracy of PDL aerosol retrievals mainly depends on their information content contained in the satellite measurements.

As shown in Figure 1, the procedure of MODIS PDL algorithm includes three major modules. First, training data sets are generated from a suite of well-designed simulations using the Unified Linearized Vector Radiative Transfer Model (UNL-VRTM) (Dong et al., 2023; Wang et al., 2014). For coarse particles, scattering kernels of spheroid aerosols with a fixed sphericity distribution are used (Dubovik et al., 2006). To obtain an effective and efficient RT simulation, we utilized aerosol optical/microphysical parameters from 7-year AERONET measurements in Beijing site during 2015–2021 and 1-year MODIS BRDF (MCD19) in eastern China during 2021 as inputs rather than random combinations of aerosol/surface parameters. There are a total of 2476 inversions of aerosol optical/microphysical parameters in Beijing site (Figures S2 and S3 in Supporting Information S1), which is influenced by anthropogenic emissions, long-range transport of airborne dust and fire smoke, and their mixtures.

The 8-day MODIS BRDF at 1 km resolution along with corresponding daily observation geometries has a huge data amount, but the statistical distributions of their values exhibit regular and slow variations (Figure S4 in Supporting Information S1). Thus, MODIS BRDF values are compressed without changing their main data features, and then are combined with the aerosol inversions randomly. At last, a total of 36,100 aerosol/surface scenarios are used for RT calculations. Since only one aerosol component model is used in each AERONET inversion, we retrieve spectral complex refractive index and effective radius and its variance of fine and coarse particles separately with an optimized method by Xu et al. (2015). Exponential-decay aerosol vertical profiles are used for fine anthropogenic aerosols, and their scale heights are set as 0.5 and 1 km in polluted days (FAOD > 0.5) during winter and other seasons, respectively (Shi et al., 2021). For coarse dust and fire smoke, central heights

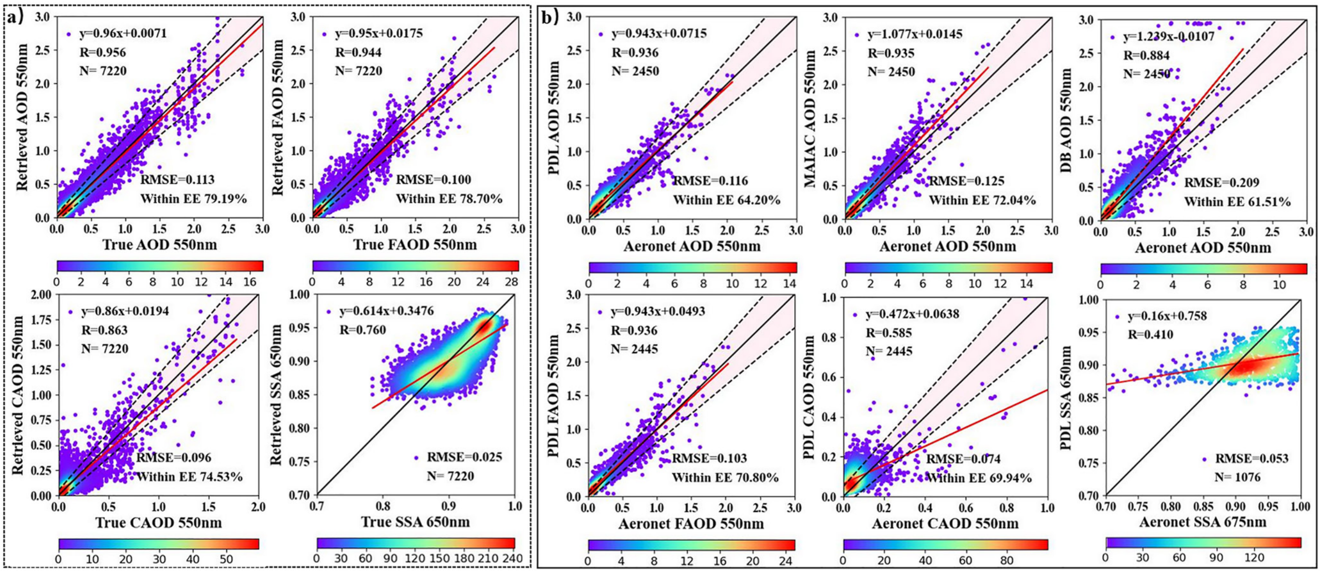

Figure 2. (a) Scatter plots of retrieved and true AOD, FAOD, CAOD at 550 nm, and SSA at 650 nm from test data; and (b) AERONET validation of corresponding MODIS PDL retrievals. The black dashed and solid lines are expected errors (EE) of ± (0.05 + 15%) and 1:1 line.

increasing with their loading are assumed in 1–3.5 km following a Gaussian distribution within 0–6 km above ground.

Spectral TOA reflectances in 1–8 spectral bands (0.4–2.1 μm) excluding the defective band 6 of Aqua MODIS are simulated by the UNL-VRTM at 36,100 aerosol-surface conditions and their associated observation geometries. Comparison of UNL-VRTM simulations with collocated AERONET observations and MODIS BRDF as inputs with single-pixel MODIS reflectance show reliable and robust performance with very high correlations in used spectral bands (R = 0.97–0.99) (Figure S5 in Supporting Information S1). The mean bias of calculated TOA reflectance ranges from −0.65% at 412 nm MODIS band with high signal-noise ratio (SNR) to −4.4% at 550 nm with much lower SNR (Figure S6 in Supporting Information S1). Then, 80% of the RT simulations is used for PDL training and the remaining random 20% as test data. Contrary to the RT simulation, the simulated satellite TOA reflectance and observation geometry are treated as inputs and aerosol parameters as outputs in the PDL training. Unlike physical retrieval algorithms that utilize absolute physical quantities, DL methods make feature learning of the whole data sets, which is not sensitive to noise.

In the second step of our algorithm, the Deep Belief Network (DBN) is utilized to establish retrieval models of MODIS AOD, FAOD, CAOD, and SSA separately. As a probabilistic generative model composed of stacked Restricted Boltzmann Machine (RBM) and a Back-Propagation net (BP), DBN has a striking advantage in modeling non-linear and high-order relationship (Hinton et al., 2006). The DBN first makes an unsupervised learning of probability distribution of the data set by the fast layer-by-layer training of each RBM. Then, a supervised fine-tuning of RBMs' weights is conducted with an error back-propagation algorithm. The two-step training process of DBN allows the learning of deep features of the data set with anti-noise capabilities.

To examine performance of trained DBN models, we make retrievals using simulated MODIS measurements from the 20% test data set and validate them with aerosol inputs as "true" values (Figure 2a). PDL retrieved AOD from simulated measurements show very accurate retrievals with high correlations (R = 0.956) and low root mean square error (RMSE = 0.113). PDL retrieved FAOD also achieves a close accuracy (R = 0.944 and RMSE = 0.1) with AOD, demonstrating that FAOD can be quantitatively retrieved by making a full use of MODIS spectral measurements. Despite a decrease in retrieval accuracy, PDL CAOD also exhibits a reliable performance with R = 0.863. Furthermore, consistent variations between PDL SSA at 650 nm and the true values (R = 0.76) show notable sensitivity of multi-spectral measurements to aerosol absorption. By applying the trained DBN models to actual MODIS measurements, we retrieve aerosols over eastern China at 1 km resolution during 2019–2021.

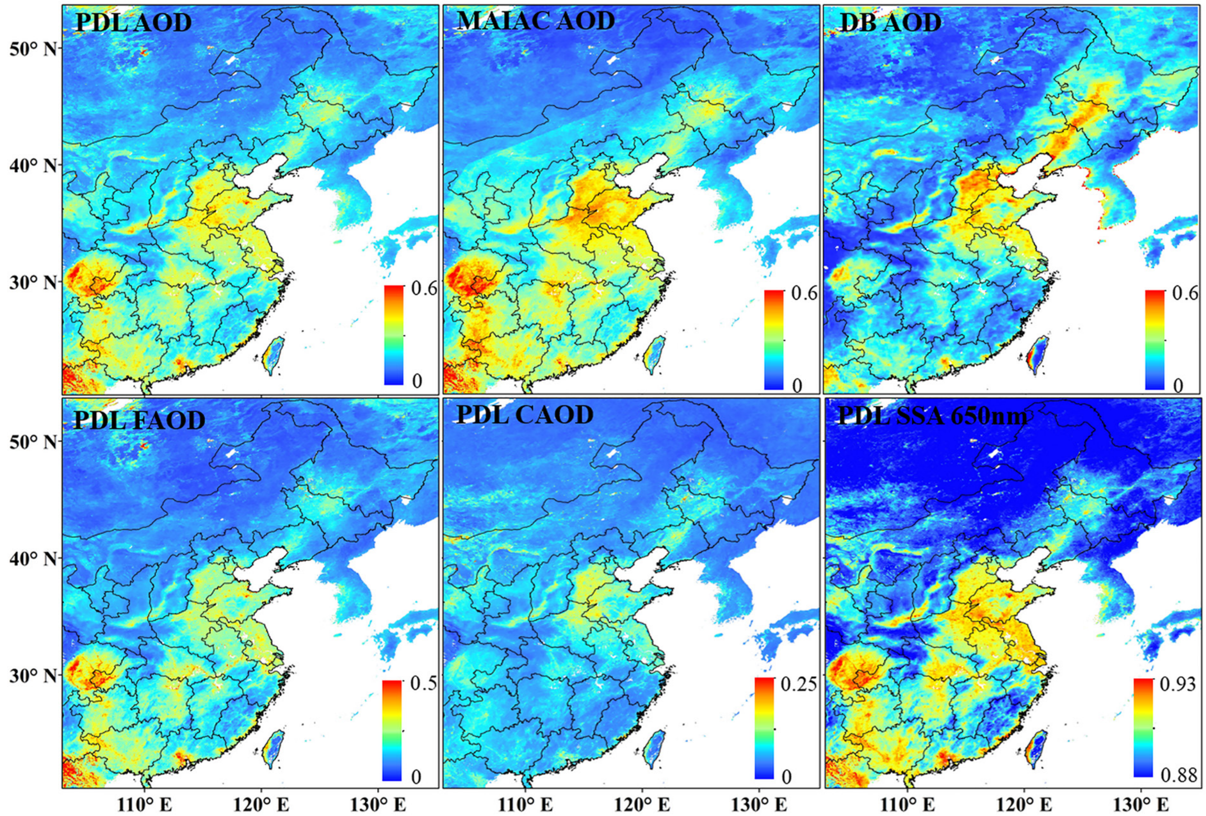

Figure 3. Annual mean of MODIS MAIAC and DB AOD, and PDL AOD, FAOD, and CAOD at 550 nm, and SSA at 650 nm in eastern China during 2021.

4. Performance and Application of MODIS PDL Aerosol Retrievals

AERONET validations show that MODIS PDL AOD (R = 0.936 and RMSE = 0.116) has very close accuracy with those retrievals from the test data (Figure 2). Moreover, PDL AOD performs better than MODIS DB products (R = 0.884 and RMSE = 0.209) over eastern China. PDL retrievals exhibit slightly higher accuracy than MODIS MAIAC AOD (R = 0.935 and RMSE = 0.125) but have less values (64.2% VS 72.04%) falling into Expected Error envelop of $\pm(0.05 + 15\%\text{AOD}_{\text{AERONET}})$. There is an obvious overestimation for PDL when AOD < 0.5, which is mainly concentrated in backscattering directions. MODIS MAIAC retrievals make a statistical correction of similar overestimation over bright surfaces in low-AOD conditions (Lyapustin et al., 2018).

The excellent performance of MODIS PDL FAOD (R = 0.936 and RMSE = 0.103) as AOD indicates that MODIS's multi-spectral measurements have sufficient information content to quantify the contribution of fine particles. The LUT-based MODIS retrievals only utilize 2–3 bands and depend on simple assumptions such as fixed aerosol types. MODIS PDL CAOD has an obviously lower accuracy (R = 0.585) than retrievals from the test data. Considering that most values of MODIS PDL CAOD is < 0.2 over eastern China, the notable overestimation can be caused by similar error sources as in AOD. Also, MODIS PDL SSA at 650 nm (R = 0.41) exhibits much poorer accuracy than the test retrieval with overestimation of low values (<0.90) and underestimation of high values (>0.90).

To further examine the performance of MODIS PDL aerosol retrievals, their annual mean over eastern China during 2021 is compared with MODIS DB and MAIAC products (Figure 3). The annual PDL and MAIAC AOD display very consistent spatial distribution at 1 km, but their magnitudes have considerable difference, especially for high values. Despite a slightly higher accuracy, MAIAC retrievals tend to overestimate high AOD values (>0.5) systematically in eastern China by utilizing one fixed aerosol model (Tao et al., 2019). By contrast, PDL AOD with reliable accuracy in high values can clearly reflect the emission hotspots in urban/industrial regions at fine scales. While high values of PDL FAOD are concentrated in anthropogenic emission sources, coarse particles with CAOD > 0.2 mainly prevail over in industrial regions of northern China and northwestern deserts.

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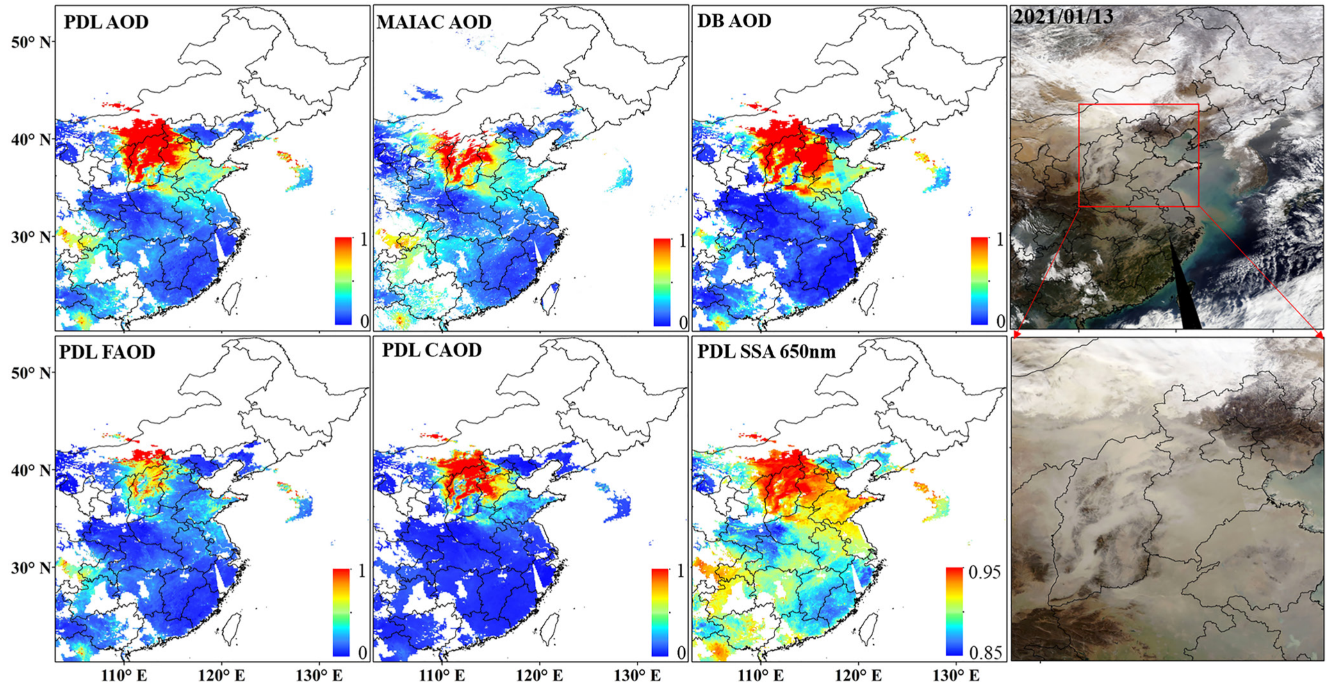

Figure 4. MODIS PDL retrievals and MODIS MAIAC and DB AOD in eastern China on 13 January 2021.

MODIS PDL SSA at 650 nm is around ∼0.88–0.89 in background regions with low-AOD, which can be unreliable due to limited information content. PDL SSA over high-AOD regions varies between ∼0.92–0.93, and aerosol absorption is relatively weak in southern China and the Sichuan Basin.

MODIS PDL retrievals are used to analyze aerosol variations during a dust event on 13 January 2021 (Figure 4). PDL, MAIAC, and DB AOD have high consistency in spatial patterns. Compared with PDL and DB AOD, MAIAC retrievals underestimate aerosol loading of the dust plumes over eastern China, due largely to fixed aerosol model with fine particles dominated. The distinct values of DB AOD in adjacent edges of the two MODIS images over northern China can be caused by bias of surface reflectance in large viewing angles. PDL CAOD clearly shows that dust particles have been prevalent over northern China before the dense dust plumes arrive in. When airborne dust is transported to downstream northern China, PDL SSA decreases from ∼0.95 to ∼0.93 with dust-pollution mixing.

PDL algorithm can make full use of not only MODIS's multi-spectral measurements, but also prior information from the existing ground-based aerosol inversions and satellite surface products. Based on the physical constraint from RT simulations, the DBN method can model the whole used spectral measurements with each retrieved aerosol parameters separately, which can avoid error propagation in optimized inversion. In particular, the PDL method has a very high computational efficiency as LUT-based retrievals. By utilizing the same forward model such as UNL-VRTM, PDL provides a unified aerosol algorithm framework for all the multi-spectral satellite measurements. With the full physical constraint from RT simulations, PDL method needs very few assumptions, and retrieval accuracy mainly depends on the information content of retrieved aerosol parameters in corresponding multi-spectral measurements. Under the unified framework, PDL algorithm can be used for aerosol retrievals from the common multi-spectral satellite instruments with different spectrum ranges and bands flexibly. As an exploratory study, here we only applied PDL algorithm for MODIS measurements over eastern China.

5. Conclusions

The widely used satellite aerosol products from spectral measurements such as MODIS only include one quantitative AOD and their retrieval uncertainties tend to be contributed by fixed aerosol models. To fully make use of the multi-spectral satellite measurements and leverage prior aerosol information from existing ground observations and satellite surface products, we developed a generalized PDL aerosol retrieval algorithm that combines the advantage of physical constraints from RT simulations and modeling ability of DL methods. By utilizing MODIS TOA reflectance at 7 spectral bands, our PDL retrievals not only have a high accuracy ($R = 0.936$) in AOD and FAOD, but also exhibit substantial consistency with AERONET observations of CAOD and SSA. In particular, PDL method has a striking computational efficiency. Based on the same forward RT model, PDL provides a unified algorithm framework for various multi-spectral satellite measurements, in which retrieval accuracy of aerosol parameters mainly depends on their information content.

Data Availability Statement

The MODIS Level 1B measurements and aerosol products are available at (MODIS science data products, 2021). The AERONET measurements and aerosol products are available at (AERONET Aerosol Team, 2019).

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