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MODIS Collection 6.1 aerosol optical depth products over land and ocean: validation and comparison

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ABSTRACT

Recently, the newest Moderate Resolution Imaging Spectroradiometer (MODIS) Collection 6.1 (C6.1) aerosol optical depth (AOD) products were available with various refinements and improvements made to both the radiation calibration and Dark Target (DT) and Deep Blue (DB) algorithms. A combined DT and DB dataset (DTB) was also added based on piecewise fixed thresholds using the Normalized Difference Vegetation Index (NDVI) for taking advantage of one's merits. This study provides a cross-comparison and evaluation of these Terra MODIS aerosol products with reference to the enhanced ground-based AOD measurements by the Aerosol Robotic Network (AERONET) Level 3 Version 2.0 data at 384 ground stations. Their absolute and relative performance are evaluated in the period of 2013–2017 among the products, as well as between the current (C6.1) and previous (C6) releases. In general, the C6.1 aerosol products are found to be superior over the C6 products for three datasets from all scales, but the differences and improvements are rather non-uniform that varies with region. Overall, the DB AOD products show the best performance in most regions at about half of the sites, especially in Europe and North America. Meanwhile, besides bright surfaces (i.e., deserts and arid/semi-arid areas), DB products match more closely with the AERONET AODs than that of DT over medium or densely vegetated areas. The dependences of retrieval errors illustrate that the performance of three datasets deteriorates as surface reflectance, elevation and aerosol loading increase. However, the DB algorithm remains relatively more stable and less affected by changes in atmospheric and surface conditions. While the merged product using NDVI has some improvements over individual ones in general, worse performance is also shown in many cases. A more optimal method is thus wanting.

1. Introduction

Atmospheric aerosols have direct and indirect effects on climate. An in-depth and better understanding of global or regional aerosol burdens is of great importance for aerosol-related studies on the ecological environment and climate change (Pöschl, 2005; Ramanathan and Carmichael, 2017; Wang et al., 2014), aerosol-cloud-precipitation interactions (Jones et al., 2010; Li et al., 2011, 2017a; Small et al., 2011), air quality and human health (Carmichael et al., 2009; Pope et al., 2002; Pöschl, 2005; Li et al., 2017b), visibility and fine particulate matter (He and Huang, 2018; Kumar et al., 2007; Xie et al., 2015; Yuan et al., 2006). Traditional ground observation sites are relatively sparse, limiting the application of these studies at medium or large scales. Moreover, aerosol loadings vary spatially and temporally.

Passive aerosol remote sensing sensors have been widely employed to retrieve aerosol optical depth (AOD) (Kaufman et al., 1997; Levy et al., 2007; Lee et al., 2009). Satellite-based aerosol retrieval always faces four major challenges including the radiometric calibration, cloud screening, surface reflectance estimation, and aerosol model assumption (Li et al., 2009; Bilal et al., 2013). The latter two remain critical and are the most important factors in radiation calculations. Different aerosol retrieval algorithms for diverse Earth-observing satellites have been developed and their strengths and limitations have been discussed (Table S1). Amon various passive satellite sensors, the Moderate Resolution Imaging Spectro-radiometer (MODIS) sensors operated on the Terra (approximately ~10:30 a.m. local time) and Aqua (approximately ~1:30 p.m. local time) have been successfully launched in December 1999 and May 2002, respectively. They have been

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extensively employed for aerosol studies with multiple aerosol retrieval algorithms, three of which are concerned in this study.

Over land, they are the Dark Target (DT) and the Deep Blue (DB) algorithms. The DT algorithm was first proposed by Kaufman et al. (1997) for densely vegetated areas based on that the surface reflectance over dark-target areas was lower in the visible channels and had nearly fixed ratios with the surface reflectance in the shortwave and infrared channels. Taking into consideration the effects of underlying surfaces and surface type, Levy et al. (2007, 2013) modified and revised the surface reflectance ratios to improve the overall accuracy of the retrievals. Confronting with the inherent limitations over bright surfaces in visible channels, Hsu et al. (2004, 2006) found that the surface reflectance for bright desert surfaces may actually be dark and stable in the deep blue channels. Taking advantage of this, they developed the DB algorithm. The third algorithm (Levy et al., 2013) was developed for oceans that is a similar but algorithmically independent DT approach. Because it considers the water from visible to longer wavelengths as dark surfaces and neglects its surface reflectance in the aerosol retrieval.

In the fall of 2017, the MODIS Collection 6.1 (C6.1) aerosol products were released based on major improvements in both radiometric calibration and all aerosol retrieval algorithms. The C6.1 aerosol products are generated based on the new updated Level 1B calibrated radiance products. It includes additional calibration corrections developed by the NASA Ocean Biology Processing Group (OBPG) that were applied to the top-of-atmosphere (TOA) radiance product of the MODIS Characterization Support Team (MCST). The MCST and OBPG corrections affect the radiometric gain, the sensor response and scan angle, and the polarization sensitivity (Jeong et al., 2011; Meister et al., 2014). The newly modified algorithms are introduced in detail in Section 2.1. Previous collections, e.g., C5, C5.1, and C6, have been extensively validated over land on local to global scales (Levy et al., 2010, 2013; Li et al., 2007; Mhawish et al., 2017; Remer et al., 2013; Sayer et al., 2015; Wei and Sun, 2017; Wei et al., 2018a). However, the C6.1 aerosol product has not been fully evaluated yet, and more importantly are the relative performance and improvement among these different products generated from the same satellite data.

Therefore, the main goal of this study is to comprehensively evaluate the new AOD products especially in terms of their relative performance among different datasets between their previous and current releases. For this purpose, we compare the three daily aerosol datasets, including the DT, the DB, and the combined DT and DB (DTB) datasets at a spatial resolution of 10 km from the Terra satellite (MOD04) during 2013–2017, against the newest release of the Aerosol Robotic Network (AERONET) Version 3 Level 2.0 ground-based AOD measurements at 384 sites around the world. Meanwhile, Terra C6 aerosol datasets for the same period are also collected for further comparison purposes. Section 2 provides descriptions of the satellite-derived products and ground observations. Section 3 describes the data matching and evaluation approaches. Section 4 presents the results of the comparisons and discusses their uncertainties. The study is summarized and concluded in Section 5.

2. Data description

2.1. MODIS aerosol products

MODIS operationally provides two kinds of long-term and global-coverage aerosol products: the Level-2 daily (swath) products at 10-km (MxD04_L2, where O is for Terra and Y is for Aqua) and 3-km (MxD04_3K) resolutions, and Level-3 daily (MxD08_D3), eight-day (MxD08_E3), and monthly (MxD08_M3) products at a $1^{\circ} \times 1^{\circ}$ horizontal resolution. The Level-3 series products are spatiotemporally aggregated from the MxD04_L2 products (Platnick et al., 2015) in which the C6.1 monthly products require valid retrievals from at least three days in a month, which is the only difference with the C6 monthly products. Except for the MxD04_3K products, all aerosol products provide three datasets: DT, DB and DTB datasets.

2.1.1. The DT dataset

The latest DT dataset is generated from the updated second-generation operational DT algorithm (Levy et al., 2013). Changes made to the C6, resulting in the C6.1 DT aerosol product, differ over ocean and land. Over ocean, standard deviation, cloud fraction, and the number of pixels for retrievals for low-AOD conditions were added in the quality control. The sediment mask was also modified to make it more robust. Over land, the quality assurance (QA) of retrievals was degraded to the lowest (QA = 0) if there were more than 50% coastal pixels or 20% water pixels in a 10 × 10-km retrieval box. The most important change was that the surface reflectance estimation model for main urban surfaces was improved (Gupta et al., 2016). The Expected Errors (EEs) are [± (0.05 + 15%)] and [± (0.03 + 5%)] for DT retrievals at a 10-km resolution over land and ocean, respectively.

2.1.2. The DB dataset

The latest DB dataset is generated by the Enhanced DB algorithm (Hsu et al., 2013) which is only applied over land. Improvements made to the C6, resulting in the C6.1 DB aerosol product, include the following over land: (1) heavy smoke detection, which can address the over-screening issue while minimizing true cloud contamination, (2) artefact reduction over heterogeneous terrain, (3) improved surface modeling for elevated terrain, and (4) bug fixes and updated regional/seasonal aerosol optical models. The EEs are approximately [± (0.03 + 21%] for 'arid' and [± (0.03 + 18%)] for 'vegetated' path DB retrievals at a 10-km resolution over land.

2.1.3. The combined DT and DB (DTB) dataset

The latest MODIS product combines the merits of the DT and DB algorithms into a new merged DT and DB aerosol dataset (DTB) that is dependent on the Normalized Difference Vegetation Index (NDVI) (Levy et al., 2013). The DTB dataset is generated as follows: (1) If NDVI > 0.3, use DT retrievals, (2) if NDVI < 0.2, use DB retrievals, (3) if 0.2 ≤ NDVI ≤ 0.3, use the average of DT and DB retrievals or the available one passing the recommended quality assurance (QA = 3 for DT and QA ≥ 2 for DB). This product increases the spatial coverage over land, especially for main transition regions which are covered by low vegetation but sufficiently dark for the DT algorithm to be applied (Levy et al., 2013). This scheme was applied for generating the DTB dataset since the C6 and no changes to the merging method have been made in C6.1.

2.2. AERONET ground-based measurements

AERONET provides long-term and freely available observations of various aerosol optical properties and spectral-deconvolution-algorithm (SDA) retrievals. The AOD observations are reported at 440, 675, 870, and 1020 nm at a high temporal resolution of 15 min with a low bias of approximately 0.01–0.02 under cloud-free conditions. They are divided into three data quality levels (L): L1.0 (unscreened), L1.5 (cloud screened), and L2.0 (cloud screened and quality assured (Holben et al., 2001; Smirnov et al., 2000). The recommended AERONET data for most previous quantitative applications has been the Version 2 L2.0 product. However, the Version 3 L2.0 database which has undergone further cloud screening and quality control is now freely available. Version 3 L2.0 data is generated based on L1.5 data with pre- and post-calibration and temperature characterization applied (Wei et al., 2017). There are four updated changes in the air mass range, the number of potential measurements, the triplet criterion, and the smoothness check, and four new added checks in very high AOD restoration, the Ångström limitation, the solar aureole radiance curvature check, and standalone points in cloud screening for the Version 3 L2.0 product (Eck et al., 2018; Giles et al., 2018). The AERONET Version 3 L2.0 product is strongly

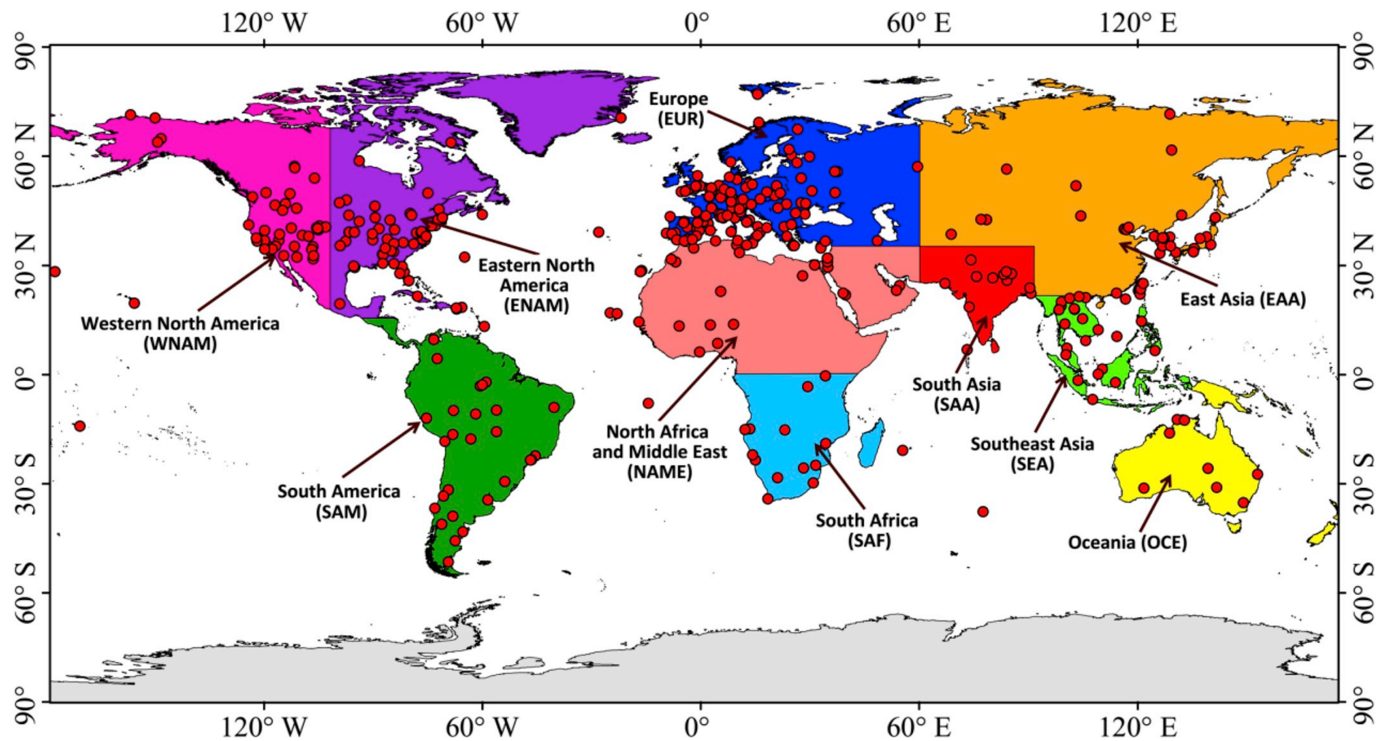

Fig. 1. Geographical boundaries of regions defined in this study. Red dots show the locations of AERONET sites. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

Table 1
Summary of data used in this study.

Product	Scientific Data Set (SDS) name	Contents	Spatial resolution
MOD04_L2	Optical_Depth_Land_And_Ocean	DT over land (QA = 3) and ocean (QA = 1,2,3)	10 km
C6/C6.1	Deep_Blue_Aerosol_Optical_Depth_550_Land_Best_Estimate	DB over land (QA ≥ 2)	
	AOD_550_Dark_Target_Deep_Blue_Combined	DTB over land and ocean	
MOD08_M3	Aerosol_Optical_Depth_Land_Ocean_Mean_Mean	DT over land (corrected)	1° × 1°
C6/C6.1	Deep_Blue_Aerosol_Optical_Depth_550_Land_Mean_Mean	DB over land (corrected)	
	AOD_550_Dark_Target_Deep_Blue_Combined_Mean_Mean	Combined DT and DB (DTB) over land	
MOD13C2	Normalized Difference Vegetation Index (NDVI)	Monthly NDVI	0.5° × 0.5°
MCD12C1	Land use cover	IGBP scheme	0.5° × 0.5°
AERONET	Version 3 Level 2.0	Aerosol optical depth	15 min

recommended for formal scientific research, so it is selected and used in this study. A total of 384 sites with more than one year of observations over land and ocean are selected (Fig. 1). Table 1 provides a summary of data used in this study.

3. Method and evaluation approaches

Terra C6.1 and C6 AODs at 550 nm with the recommended QA for the DT (QA = 3 for land and QA = 1, 2, 3 for ocean), DB (QA ≥ 2), and merged DTB products (QA = 3) at a 10-km resolution are simultaneously selected. The retrievals were defined as average values within sampling windows with 3 × 3 pixels (at least 3 out of 9 pixels available) centered on the AERONET site. The average of at least two AERONET AOD measurements within 1h (± 30 min) of the Terra overpass time defined the “true” value (Wei et al., 2017, 2018a,b). AERONET sites do not provide AOD retrievals at 550 nm, therefore, the Ångström algorithm (α) in 440–675 nm was selected to interpolate AOD values at 550 nm using the available AOD measurements at the nearest wavelength (λ) of 500, 440, or 675 nm (Sun et al., 2015; Wei et al., 2017, 2018a,b). Statistical tools and techniques used to quantify the accuracy and uncertainty of the different aerosol datasets against AERONET ground measurements include the Pearson product-moment correlation coefficient (R), the Mean Absolute Error (MAE), the Median Bias (MDB), the Root-Mean-Square Error (RMSE), and EE (Eq. (2)) of the DT algorithm.

$$AOD_{550} = AOD_{\lambda}(550/\lambda)^{-\alpha} \tag{1}$$

$$EE = \pm(0.05 + 0.15{*}AOD_{AERONET}) \tag{2}$$

4. Results and discussion

4.1. Spatial distributions and variabilities among aerosol datasets

First, we focus on examining regionally and globally aggregated C6.1 and C6 data to examine their similarities and differences. For this purpose, the spatial distributions and differences among the three datasets derived from the two collections are averaged from the Level-3 MOD08_M3 monthly aerosol products from 2013 to 2017. Fig. 2 shows the 5-years averaged DT, DB, and DTB AODs and their differences between C6.1 and C6 releases over land and ocean. The corresponding statistics of annual mean aerosols are given in Table S2.

Over ocean, the spatial coverage of C6.1 DT is slightly narrower than that of C6 DT along land-sea borders and a few inland areas mainly because the QA was degraded to 0 if there were more than 50% coastal

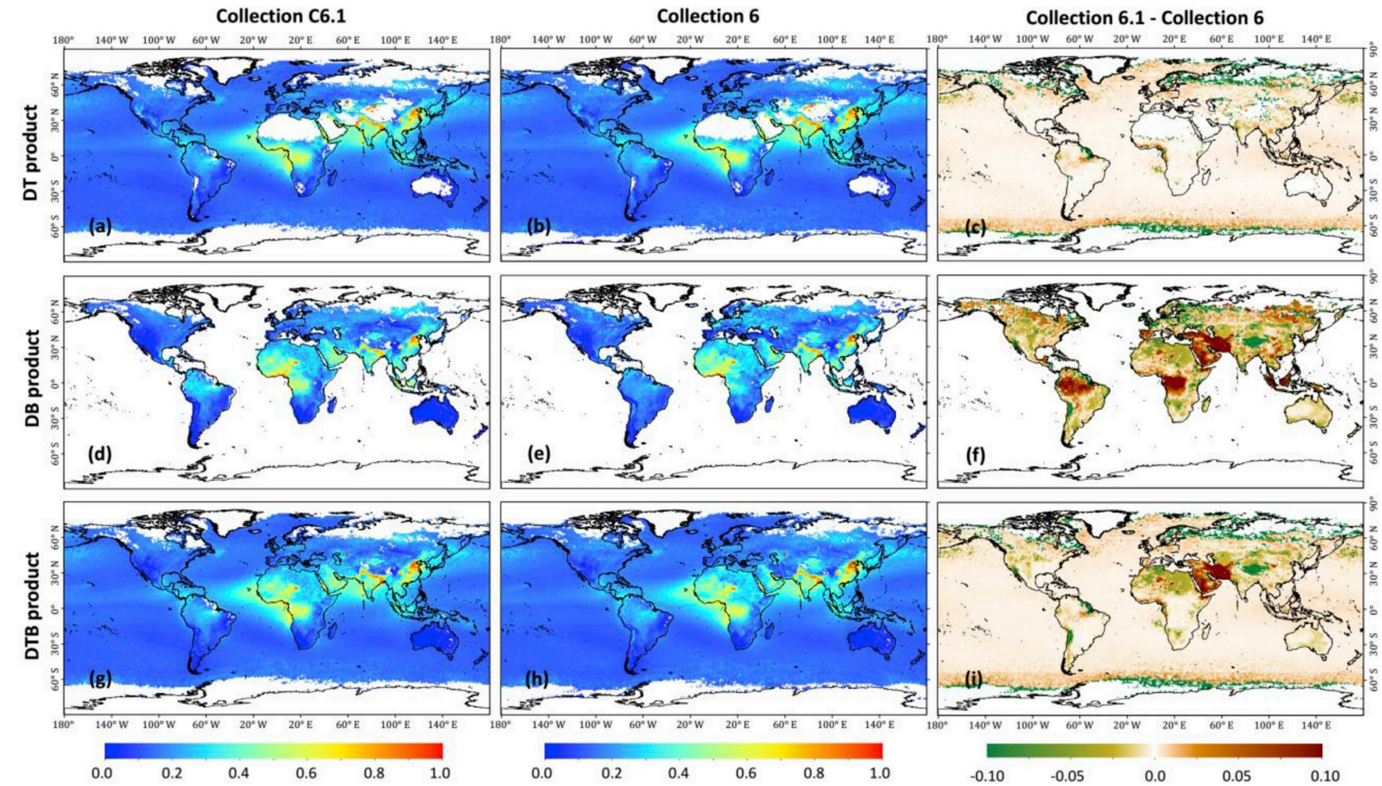

Fig. 2. Spatial distributions of annual mean AODs for Terra MODIS C6.1 DT, DB, and DTB datasets (left panel from top to bottom), Terra MODIS C6 DT, DB, and DTB datasets (middle panel from top to bottom), and differences between the Terra MODIS C6.1 and C6 DT, DB, and DTB datasets (right panel from top to bottom). Data are from 2013 to 2017.

pixels or 20% water pixels in the retrieval box. The annual mean C6.1 DT AOD is 0.162 ± 0.07 which is slightly larger than that of C6 DT AOD (0.159 ± 0.07) over ocean. There are no clear differences between two collections over the main oceans.

Over land, these aerosol datasets show similar spatial distributions with annual mean AODs of ~0.22 ± 0.15. High aerosol loadings are mainly found over North Africa and the Middle East, South Asia, and East Asia, while low aerosol concentrations are widely distributed throughout the rest of the land areas. The DT product shows a large number of missing values in most arid and desert areas concentrated over North Africa, the Middle East, central Asia, and Australia due to the limitations of the DT algorithm. However, the DB algorithm can provide almost complete land coverage over both dark and bright surfaces.

Differences will arise in the datasets as updates to the algorithms are made. C6.1 DT retrievals are overall lower than C6 DT retrievals over India and parts of Asia, by contrast, positive differences between them are found over Europe and western Africa. However, there are no significantly differences in most land areas (Fig. 2c). There are significantly differences between the C6.1 and C6 DB datasets at the regional level, where the positive differences are observed over Southeast Asia, the Middle East, northern South America, and central Africa. By contrast, the negative differences are found over Europe, North, northern Africa and central Asia (Fig. 2e). For C6.1 and C6 DTB datasets, significantly positive differences are observed over the Middle East, while negative differences are found over North Africa, western North America, and central Asia (Fig. 2i). Such differences may be resulted from the improved aerosol estimations with many improvements of the DB algorithm over land.

Fig. S1 shows annual mean differences between the C6.1 and C6 DT and DB, DT and DTB, DB and DTB products from 2013 to 2017 over land. In general, there are significant differences between the DT and DB products. Except for DT-algorithm-restricted arid and desert areas, significantly positive differences are observed over Eastern Europe and South America. DB retrievals are much lower than DT retrievals over western North America, central Africa, East and South Asia. There is no significantly difference between the DTB and DT AODs over most areas, suggesting that the DTB algorithm selects mainly DT retrievals over these areas. Significantly positive differences are seen in main arid and desert areas because the DT algorithm is not applicable there, so the DTB algorithm selects DB retrievals over these areas. In addition, significant negative differences are mainly observed over semi-arid and mountainous areas, i.e., western North America, southern South America, and the Middle East. For DTB and DB datasets, significantly positive differences are observed in western North America, central Africa, East and South Asia, yet negative in southern Sahara Desert and Eastern Europe. The limitations of the individual algorithms over different underlying surface types likely account for the noticeable differences among these three products.

4.2. Validation and comparison with AERONET measurements

4.2.1. Global-scale analysis

Fig. 3 presents the validations of Terra C6.1 DT, DB, and DTB retrievals against AERONET AOD measurements at 34 sites over ocean and 350 sites over land from 2013 to 2017, respectively. Note that the marine ground-based observation sites are relatively few and they are mainly located in coastal waters. For ocean, the C6.1 DT AODs agree well with AERONET AODs (R = 0.880, MAE = 0.055, and RMSE = 0.083) with 73.5% of the data samples fall within the EE envelopes (Fig. 3a). The C6 DT AODs (Fig. S2a) show similar performance (R = 0.883, MAE = 0.056, and RMSE = 0.085) with the C6.1 DT AODs over ocean. However, the C6.1 DT sample size is smaller than that of C6 DT because of the reduced quality assurance of retrievals if there are more than 50% coastal pixels in a 10 × 10-km retrieval box.

For C6.1 DT AOD retrievals over land (Fig. 3b), the matched

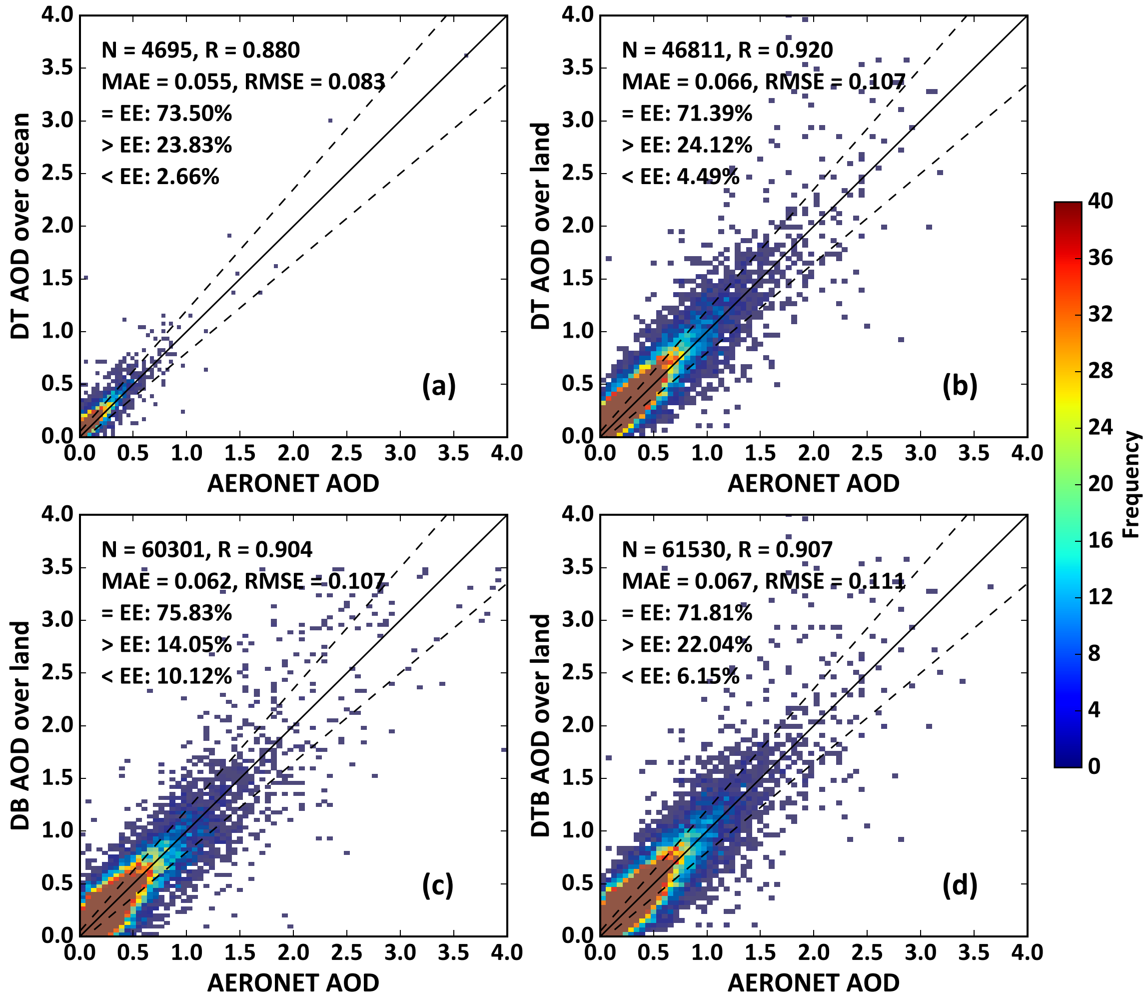

Fig. 3. Density scatter plots of Terra MODIS C6.1 DT over ocean (a), DT (b), DB (c) and DTB (c) AOD retrievals over land against AERONET AOD measurements from 2013 to 2017. The solid line denotes the 1:1 line, and the dashed lines denote the envelopes of the expected error (EE). The sample size (N), correlation coefficient (R), mean absolute error (MAE), and root-mean-square error (RMSE) are also given. Note =/ > / < EE represent the percentages (%) of retrievals falling within, above, and below the EE, respectively.

samples are collected from 336 sites and the remaining 14 sites are mainly distributed in arid/semi-arid and desert areas where the DT algorithm cannot be applied. C6.1 DT AOD retrievals show good agreements with AERONET AODs (R = 0.920) and 71% of the points fall within the EE envelopes, along with an average MAE of 0.066 and RMSE of 0.107. There are ~29% more samples from the C6.1 DB dataset than from the C6.1 DT datasets over land (Fig. 3c). C6.1 DB AOD retrievals agree slightly less with AERONET AOD measurements (R = 0.904) but with a higher percentage of points fall within the EE envelopes (76%) and a smaller mean MAE (0.062) compared to C6.1 DT AOD retrievals. C6.1 DTB AOD retrievals agree well with ground measurements (R = 0.907) with an average MAE of 0.067 and RMSE of 0.111. The percentage of points falling within the EE envelopes on a global scale is 72% (Fig. 3d). For land, in general, the C6.1 DT, DB and DTB products are overall better with increasing fractions of the points matching in the EE envelopes by approximately 7%, 5% and 7% and decreasing estimation uncertainties (i.e., MAE and RMSE) than the corresponding C6 aerosol products, respectively (Figs. S2b, c, d). These results mainly result from the continuous improvements made to their respective aerosol retrieval algorithms.

4.2.2. Regional-scale analysis

Due to the changing geography, climate, and human activity, differences may arise for different aerosol products at the regional levels. Therefore, regional analyses are done for the ten custom regions (Table 2). Over East Asia, DB retrievals show the best performance with all the best statistical metrics among the three datasets. The DT algorithm significantly overestimates the aerosols with 32–38% of the points falling above the EE envelopes. The main reason is that most areas are arid/semi-arid or densely populated urban areas facing complex surface structures, which limit the application of DT algorithm. Similar performance is seen for DTB retrievals. Over South Asia, DT and DTB retrievals are similar in accuracy with almost the same statistical metrics. By contrast, DB retrievals show the worst performance and significantly underestimate the aerosols due to the overestimation of surface reflectance (Mhawish et al., 2017). Over Southeast Asia, DT and DTB retrievals show similar performances because DTB product mainly selected the DT retrievals (Fig. S1c). By contrast, DB shows poor performance with only 49–52% of points falling within the EE envelopes. This contributes to the inaccurate estimation of surface reflectance.

Over Europe, AOD retrievals from the three datasets agree well with ground measurements and about 67–83% of all points fall within the EE envelopes with RMSE values less than 0.08. The main reason is that the dense vegetation coverage allows for more accurate estimations of surface reflectance. DTB and DT retrievals are similar according to their statistical metrics. This is because in most areas, the DTB algorithm selected the DT AOD retrievals (Fig. S1c). However, DB retrievals shows the best performance with all the best statistical metrics.

Over Eastern North America, three datasets are high related to

Table 2
Statistics describing the relationships between Terra C6.1 DT, DB, and DTB AOD retrievals and AERONET AOD measurements for each region from 2013 to 2017.

Region	N			R			MDB			RMSE			Within EE (%)		
	DT	DB	DTB	DT	DB	DTB	DT	DB	DTB	DT	DB	DTB	DT	DB	DTB
EAA	4363	4935	5698	0.931	0.942	0.936	0.045	0.017	0.040	0.144	0.134	0.144	63.5	69.4	66.0
SAA	2161	2272	2462	0.874	0.870	0.868	0.011	−0.087	−0.007	0.185	0.219	0.187	66.9	48.9	62.1
SEA	2243	1904	2244	0.905	0.890	0.905	0.025	−0.002	0.025	0.198	0.191	0.198	61.6	51.6	61.6
EUR	15276	15286	15621	0.845	0.831	0.845	0.029	−0.002	0.029	0.078	0.062	0.078	73.5	82.5	73.6
ENAM	8242	9591	8490	0.937	0.857	0.919	0.016	0.011	0.015	0.059	0.076	0.062	83.3	82.2	82.2
WNAM	6492	10179	10131	0.818	0.868	0.815	0.043	−0.005	0.018	0.113	0.089	0.093	59.6	85.1	74.4
SAM	3135	3684	3686	0.925	0.940	0.939	0.019	−0.001	0.008	0.084	0.057	0.070	71.3	85.7	83.0
NAME	1838	8110	8515	0.909	0.849	0.838	0.005	0.023	0.026	0.142	0.156	0.155	66.2	55.7	56.1
SAF	1212	1767	1965	0.906	0.786	0.843	−0.015	−0.022	−0.011	0.092	0.101	0.099	74.4	71.5	72.1
OCE	1300	2409	2162	0.523	0.490	0.501	−0.001	−0.017	−0.003	0.066	0.052	0.060	85.4	83.5	85.3

ground measurements and have 76–84% of the points falling within the EE envelopes with low bias and RMSE values. The main reason is that Eastern North America has dense vegetation coverage with low surface reflectance like Europe and the DTB algorithm mostly selected the DT AOD retrievals (Fig. S1c). DB retrievals show the best performance with all the best statistical metrics. However, the DT algorithm performs poorly over western North America due to complex terrains with high surface reflectances. The retrievals have great uncertainties with large positive biases and RMSE values, suggesting significant overestimations. By contrast, the DB algorithm performs much better with 44–58% more data points and better statistical metrics than the DT algorithm. Note that the DTB products are much better than the DT products but less accurate than the DB products.

Over South America, three datasets show good performances, and about 67–86% of the retrievals fall within the EE envelopes with low bias and RMSE values. The abundant tropical rainforests at the central and northern South America allow for better AOD retrievals. Over Oceania, the land cover varies from east (dense-vegetation areas) to west (deserts and arid/semiarid areas). Thus, less samples are collected from DT products, and 83–86% of them fall with the EE envelopes. By contrast, the DB algorithm can retrieve 1.7–1.9 times more AODs than the DT algorithm with more than 82% of the data points falling within the EE envelopes. In addition, DTB retrievals show similar performances with DB products.

Over North Africa and Middle East, the DT algorithm generally fails because of the bright desert surfaces (sample size = 1800). The DB algorithm provide more than four times samples than the DT algorithm due to improved surface reflectance estimation. The DTB and DB retrievals are similar because the merging procedure chooses DB retrievals. Due to the extremely high surface reflectance, the sensitivity of aerosol changes to apparent reflectance decreases (Sun et al., 2015; Wei et al., 2018a,b). Meanwhile, varying composition of aerosols also makes retrieving AOD difficult. Thus, DB and DTB retrievals have large RMSE values (> 0.15) and low percentages of points falling with the EE envelopes. Over South Africa, there are more vegetation and all three algorithms perform well with more than 69% of all data points falling within the EE envelopes. The bias and RMSE values are generally less than 0.02 and 0.1, respectively.

In general, the DT algorithm is more suitable for highly vegetated areas in Europe, Eastern North America and South America. A greater number of DTB AOD retrievals are generated over most regions which have similar statistical metrics as the DT AOD retrievals except for bright surfaces. The DB algorithm performs the best in most regions over both dark-target and bright surfaces. There is no doubt that the DB algorithm is the most appropriate choice for applications for bright arid and desert areas (i.e., North Africa, Middle East, central Australia, central and eastern Asia) where DT coverage is missing. In general, C6.1 AOD products are an improvement upon C6 AOD products on regional scales, especially for Asia, Europe, North America (Table S3).

4.2.3. *Site-scale analysis*

Aggregated global and regional statistics primarily provide a picture of the overall performance for different aerosol products. However, it may cause a certain uncertainty due to the inhomogeneity of AERONET sites across the world or within a region and the different sample sizes among sites, meaning that sites are not weighted equally in combined metrics. Therefore, further detailed validations are performed at the AERONET-site scale. Fig. 4 presents the validation of Terra C6.1 DT, DB, and DTB AOD retrievals against AERONET AOD measurements for all individual sites from 2013 to 2017. For statistical significance, only sites with at least 20 match-ups (three-way DB/DT/DTB) are used. Those sites where an algorithm provides few or no retrievals are marked as black dots. Site-scale validation allows to show which algorithm does the best at each individual site.

C6.1 DT retrievals agree well with AERONET AOD measurements at most sites around the world. More than 73% of the sites have correlations greater than 0.8, especially in Asia, eastern North America, northern South America and Europe. Sites with low correlations are found in Western North America, and central Australia. Approximately 58% of the sites having more than 70% of samples falling within the EE envelopes. These sites are mainly distributed in Eastern North America, Europe, and the Amazon region. The DT algorithm overestimates AOD at most sites around the world, especially in Asia and Western North America. Underestimations of AODs are found at the sites in Africa. RMSE values are less than 0.08 at 54% of the sites in the world, especially in eastern North America and Europe. Sites with larger RMSE values are distributed throughout central Africa and Asia.

C6.1 DB retrievals shows similar spatial variations in correlations with ground measurements at most sites over land to the DT retrievals. Fifty-eight percent of the sites have correlations greater than 0.8. Sites with more than 70% of data points falling within the EE envelopes are observed at 64% of the sites on land, especially for North America, South America, and Europe. Some individual sites located in Africa and Asia have low numbers of points falling within the EE envelopes. Forty-seven percent of all sites have small biases (~-0.02–0.02). DB AODs are overestimated at some sites in North Africa, Middle East, Southeast Asia, and East Asia. By contrast, large underestimations are found at some sites in South Asia and Africa. Small RMSE values are found at most North American, South American, and European sites, but large RMSE values are seen at African and Asian sites. However, ~55% of the sites have RMSE values less than 0.08 over land.

C6.1 DTB retrievals show similar spatial patterns but numerical differences of the four statistical metrics with the DT AODs at most sites around the world. In general, Seventy-three percent, 41%, 58%, and 63% of the sites have high correlations (R > 0.8), high fractions of points within the EE envelopes (> 70%), small median biases (~-0.02–0.02), and small RMSEs (< 0.08), respectively. The DTB retrievals have more data points within the EE envelopes, smaller median biases and RMSEs than the DT retrievals over those areas where DT algorithm performs poorly, i.e., western North America, North America,

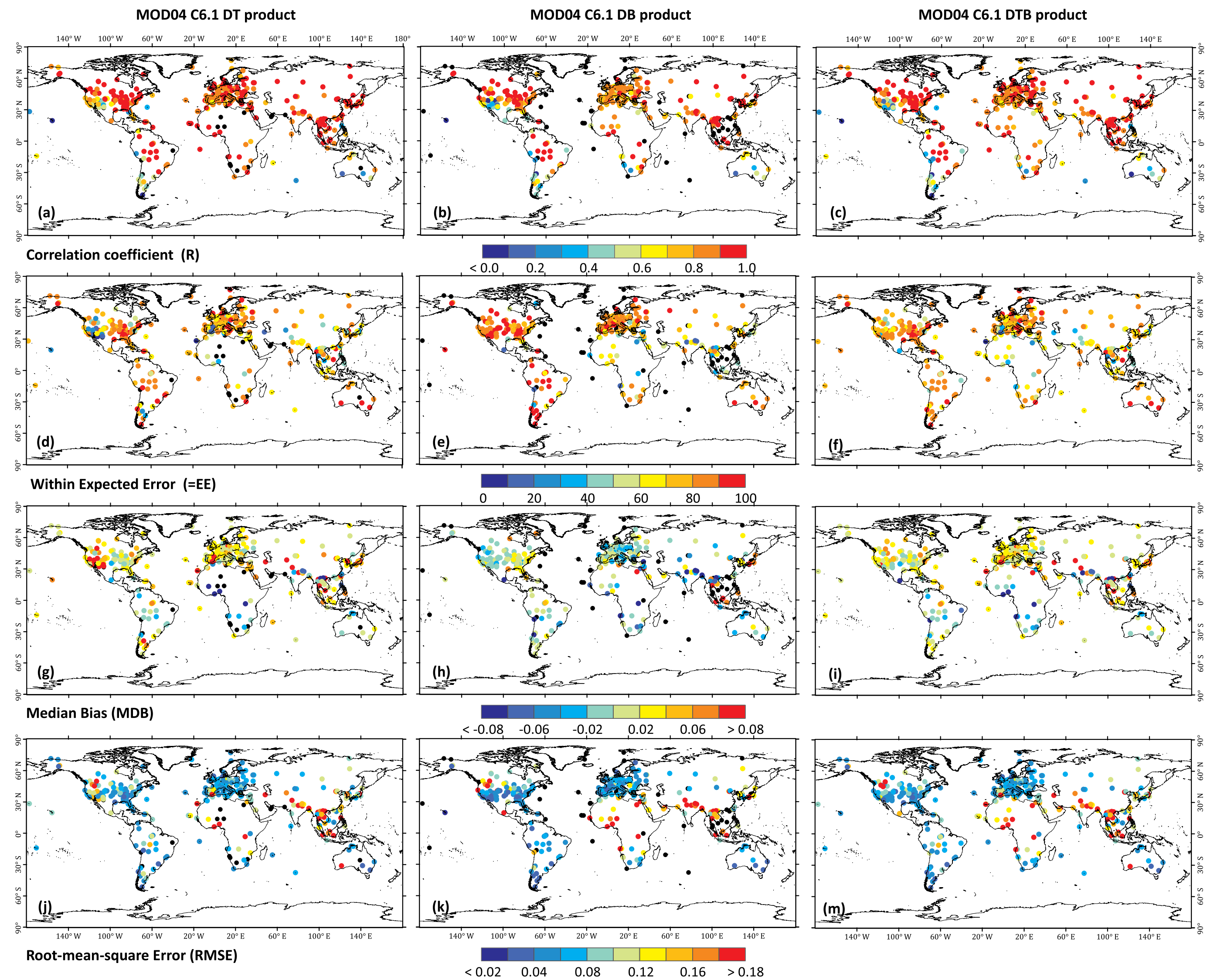

Fig. 4. Validation of Terra MODIS C6.1 DT, DB, and DTB AOD retrievals against AERONET AODs for each site from 2013 to 2017: (a–c) correlation (R), (d–f) percentage of retrievals within the expected error envelopes (%), (g–i) median bias, and (j–m) root-mean-square error.

North Africa and the Middle East.

Site-scale C6 aerosol products were also validated using the same approach and similar results were obtained for the C6 DT, DB, and DTB products (Fig. S3). In general, C6.1 DT product performs better at ~66% of sites in fractions matching the EE envelopes, ~50%, ~62% and ~60% of the sites in terms of R, bias, and RMSE than C6 DT product, respectively. In addition, C6.1 DB product shows better performances at ~60%, ~61%, ~56% and ~51% of the sites in terms of fractions matching the EE envelopes, R, bias and RMSE than C6 DB product, respectively. For merged products, C6.1 DTB product shows improvements in ~51%, ~67%, ~61% and ~59% of the sites in terms of fractions matching the EE envelopes, R, bias, and RMSE compared to C6 DTB product, respectively (Figs. S4 and S5). However, there are small differences in the performances for two collections in the rest sites. These results indicate that the data quality of the C6.1 products has generally improved on the site scales.

Fig. 5 shows the algorithm that performs the best at each site for four selected evaluation metrics, including the highest number of retrievals, the highest fraction of points within the EE envelopes, the lowest absolute median bias (note that absolute bias is used rather than the difference in bias itself as a "better" comparison will have a bias closer to zero), and the lowest RMSE. The DT algorithm shows the best performance in all metrics at only a few sites on land. The DB algorithm has the best performance at a large number of sites with the highest number of retrievals (52% of the sites), the highest fraction of points falling within the EE envelopes (49% of the sites), the lowest bias (48% of the sites) and RMSE (47% of the sites) values. These sites are concentrated in North America, Europe, and South America. The DTB algorithm generates the largest number of retrievals in western Northern America, South Asia, and Mediterranean coastal areas. The DTB and DT algorithms perform equally well at 33% of the sites located in Europe, Eastern North America, and Southeastern Asia. Although the DTB algorithm takes advantage of both DT and DB retrievals, it does not perform as well as the DB algorithm at approximately half of the selected sites. This suggests that the DTB products based on independent NDVI data are not always the best among three datasets at the site scale. The same evaluation was done on C6 aerosol products (Fig. S6). Aside from differences in the proportion of sites where algorithms performed the best, results similar to those for C6.1 are found (Table S4).

4.3. Discussion and uncertainty analysis

In this section, we focus on the performance and uncertainty of three aerosol products related to several main factors (including the

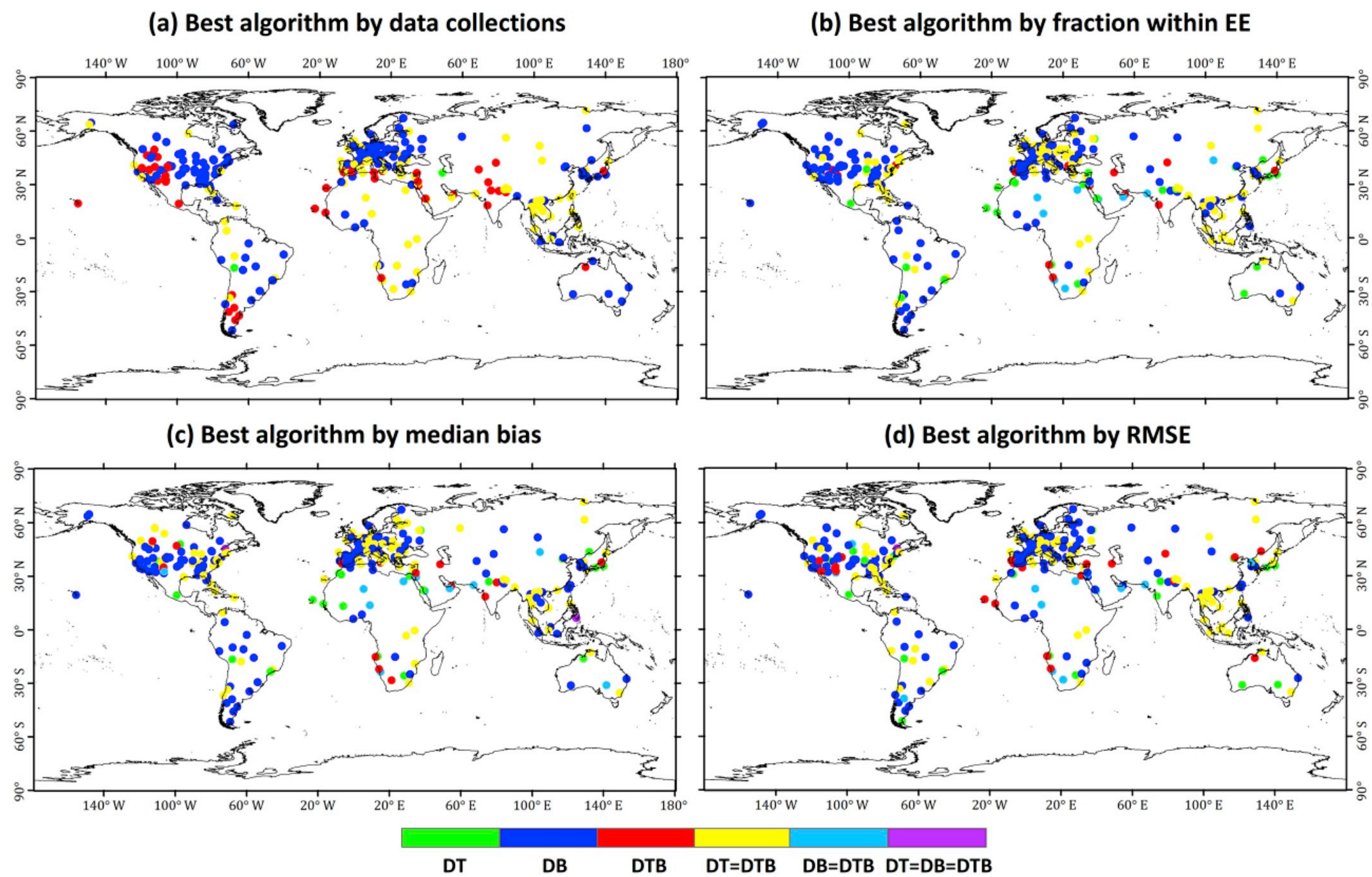

Fig. 5. Geographical distribution of sites showing where the MODIS DT, DB, and DTB algorithms performed best on land according to different statistical metrics: (a) the number of retrievals, (b) the percentage of points falling within the EE envelopes, (c) the median bias, and (d) the root-mean-square error (RMSE).

surface reflectance, aerosol type, pollution level, elevation, NDVI and land use types) affecting the aerosol retrieval. For this purpose, according to the MODIS surface reflectance (MOD09, Vermote and Vermeulen, 1999; Sun et al., 2016a,b; Wei et al., 2018b), aerosol (MOD04, Sun et al., 2016b; Wei et al., 2018b), NDVI (MOD12) and land use cover (MCD13) products and AERONET ground measurements, three aerosol products for two collections are divided into several groups and validated against the ground measurements. Figs. 6–9 show the box plots of the distributions of the performance and errors among C6.1 and C6 DT, DB, and DTB retrievals as a function of land surface reflectance and aerosol type, pollution level, elevation, NDVI and land use types, respectively. The results show that the distributions of and variations between the different aerosol datasets from C6.1 and C6 versions are similar. For the same algorithm-generated datasets, the C6.1 products are overall better than the C6 products for most conditions.

4.3.1. Uncertainty related to surface reflectance and aerosol type

All datasets perform well over darker surfaces (LSR $\leq$ 0.05, Fig. 6a and b). The DT retrievals have large positive biases, while the DB biases are closer to 0, indicating a better performance. The DTB and DT biases are similar but overall worse than DB in terms of the percentage of retrievals falling within the EE envelopes. For 0.05 < LSR < 0.10, the DT performance sharply declines with increasing positive biases. By contrast, the DB algorithm performs better with a higher percentage of retrievals falling within the EE envelopes and smaller biases. The performances of the DTB and DB algorithms are consistent and much better than the DT algorithm. For brighter surfaces (LSR $\geq$ 0.10), although the DT algorithm seemingly performs well, its application is largely limited with few successful retrievals. By contrast, the DB algorithm can provide four times more retrievals than the DT algorithm. However, DB retrievals are more tightly clustered around the bias equal to 0 with higher fractions of retrievals within the EE envelopes, suggesting a much better performance than the DT algorithm under changing surface reflectance conditions. In general, the performances of all datasets decrease gradually as LSR increases due to the decreasing sensitivities of aerosol changes to apparent reflectance (Wei et al., 2018a,b).

The DT algorithm performs well in these areas where strongly, moderately, and weakly absorbing aerosols dominate (Fig. 6c and d). However, its performance deteriorates in areas where continental and dust aerosols dominate, i.e., the interior parts of the continents and deserts. The DB algorithm performs better than the DT algorithm in areas where moderately and weakly absorbing aerosols and continental aerosols dominate. Its performance deteriorates in areas with strongly absorbing aerosols, i.e., southwestern South America, South Africa, and Southeast Asia. The quality of the DTB and DT retrievals in areas where strongly, moderately, and weakly absorbing aerosols dominate are similar. All the algorithms perform generally poorly in dust-dominated areas because of the difficulty in generating aerosol retrievals due to high-reflectance surfaces and changing optical properties (i.e., single scattering albedo and asymmetry factor).

4.3.2. Uncertainty related to pollution level

In general, all datasets worsen as the aerosol loading increases (Fig. 7). For slightly polluted cases (AOD $\leq$ 0.5), DT retrievals show good performances with more than 60% of them falling within the EE envelopes but with large positive biases greater than 0.025. DB retrievals have an overall lower percentage falling within the EE envelopes, but more stable biases closer to zero than DT retrievals. Similar distributions and variations are found between DTB and DT retrievals. For moderately polluted cases (0.5 < AOD < 1.0), 55–66% of all retrievals fall within the EE envelopes. DT retrievals still show large

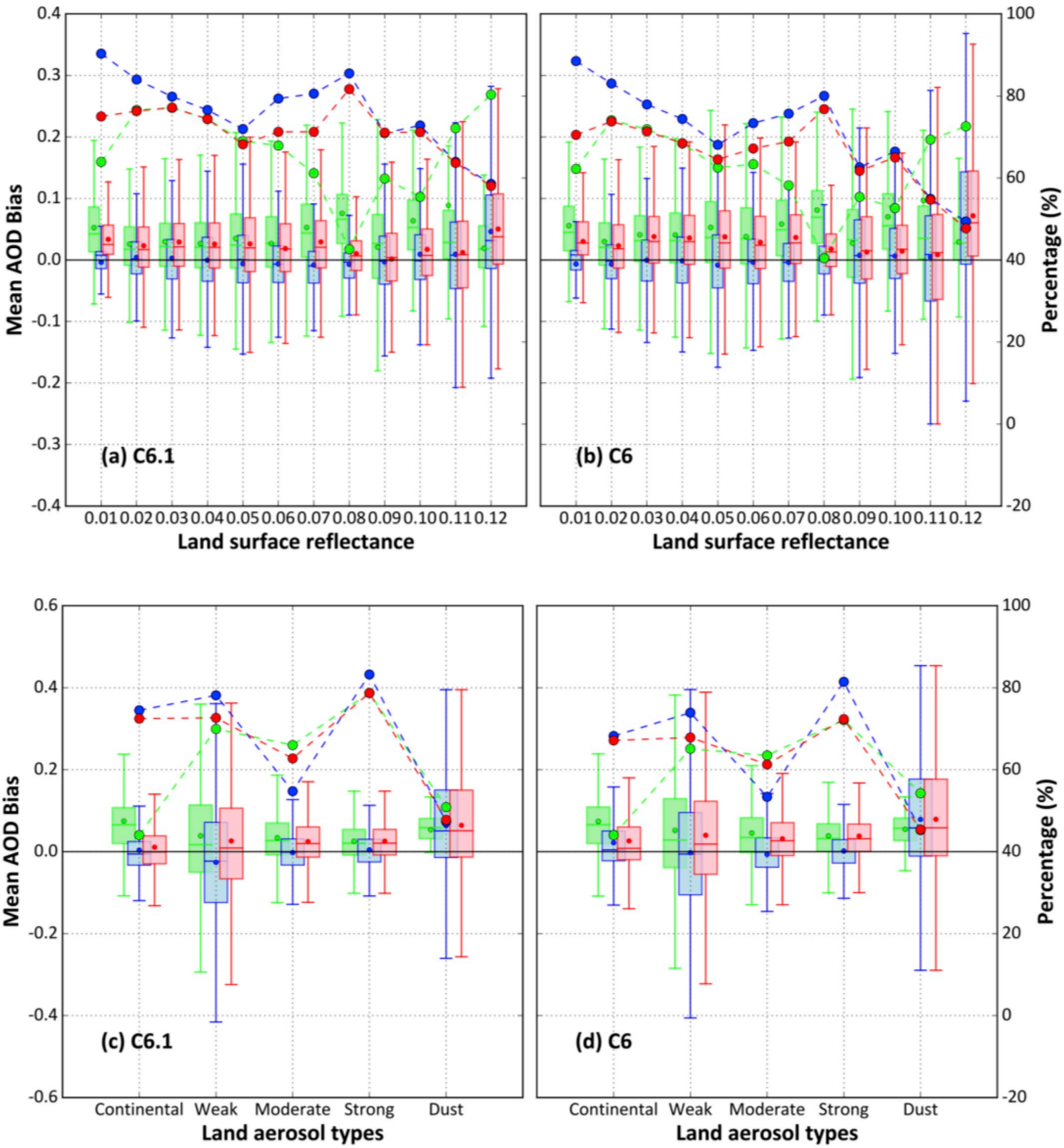

Fig. 6. Box plots of AOD bias and the percentage of retrievals falling within the EE envelopes (curves) for MODIS C6.1 (a, c) and C6 (b, d) DT, DB and DTB AOD retrievals against AERONET AOD measurements as a function of surface reflectance (a, b) and aerosol type (c, d). Green, blue, and red represent DT, DB, and DTB results, respectively. The black horizontal solid line represents the zero bias. In each box, the middle, lower, and upper horizontal lines represent the AOD bias median, and 25th and 75th percentiles, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

positive biases around 0.026, while the DB biases become more negative as AOD increases. DTB retrievals have smaller biases closer to 0 than do the DT and DB retrievals. For heavily polluted cases (AOD ≥ 1.0), all datasets have large biases and decreasing percentages of retrievals falling within the EE envelopes. The number of DT retrievals is much less than that of the DB retrievals, yet the DB retrievals show large underestimations. This suggests that aerosol retrievals under heavily polluted conditions still face great challenges.

4.3.3. Uncertainty related to ground elevation

In low-elevation areas (Height, H < 800 m), all three datasets show good performances with small biases and high percentages of retrievals falling within the EE envelopes (Fig. 8). However, in these areas, the retrieval uncertainty mainly related to other true aerosol-influential

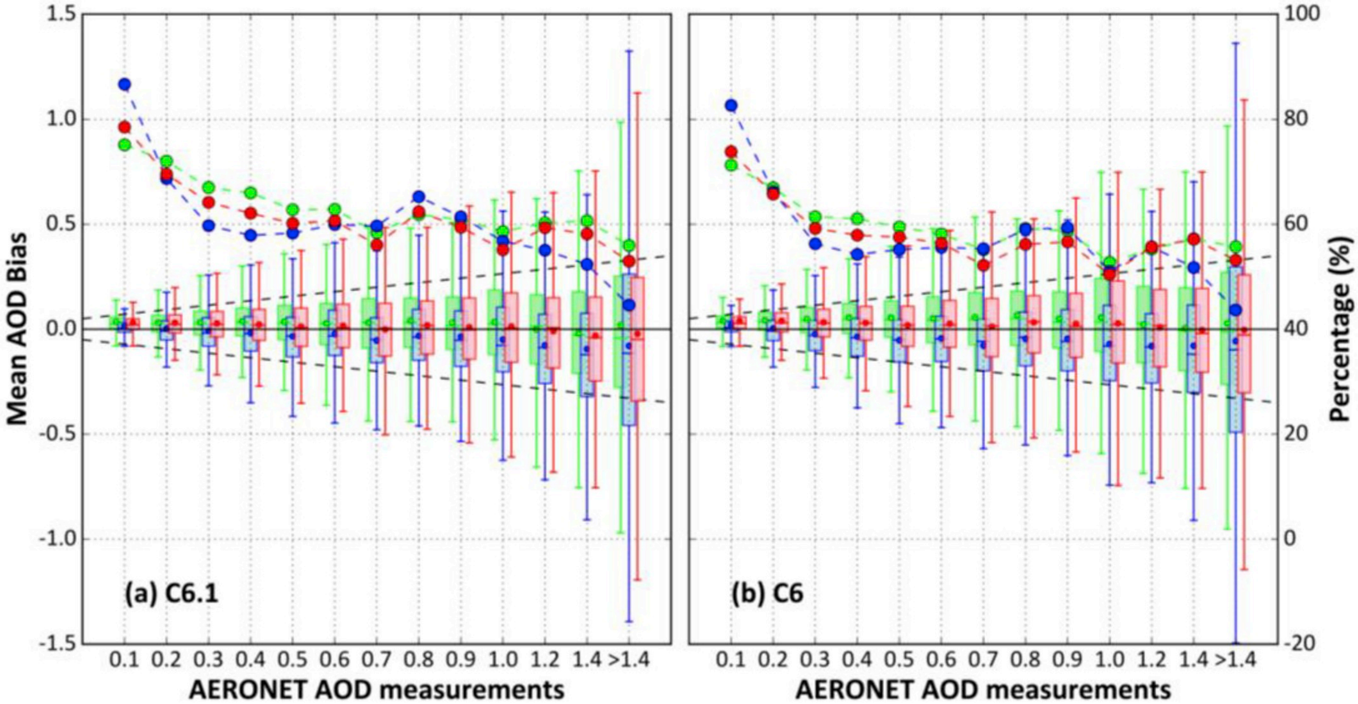

Fig. 7. Same as Fig. 6 but as a function of pollution level.

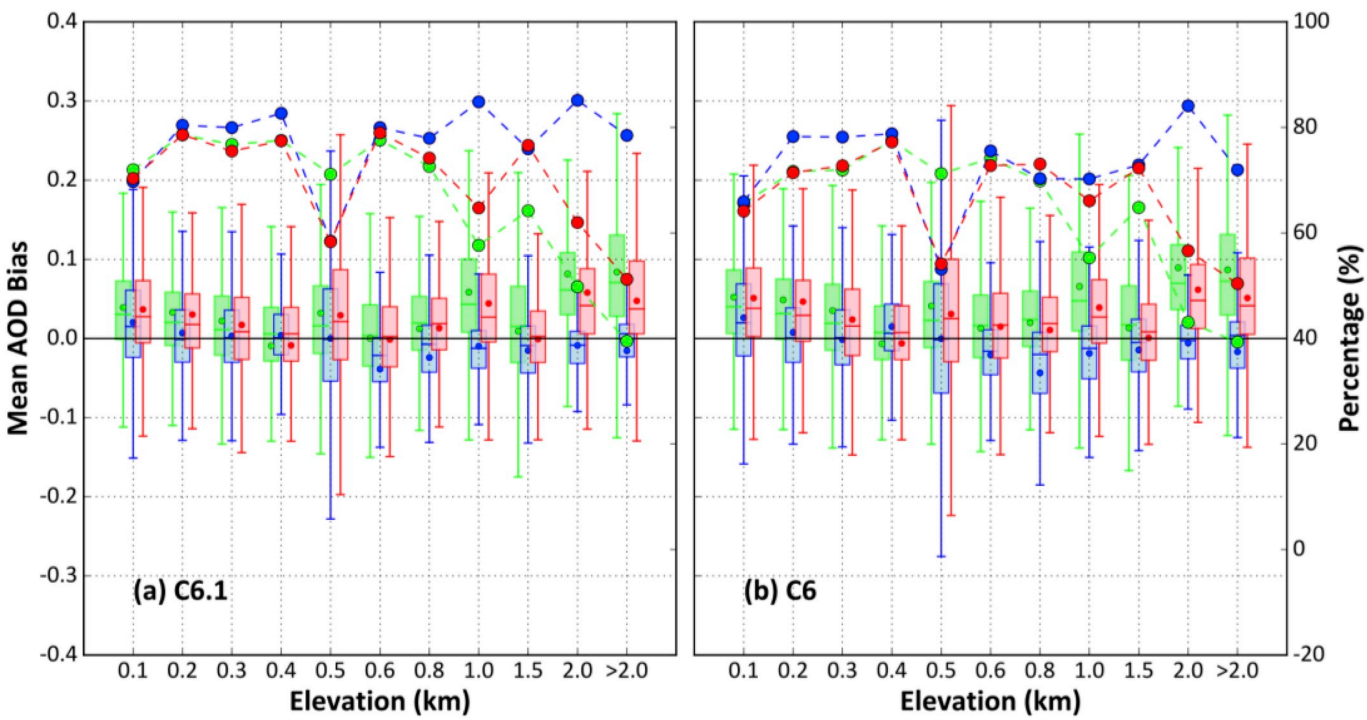

Fig. 8. Same as Fig. 6 but as a function of ground elevation.

factors. Thus, we mainly focus on high-altitude areas. It is found that the DT retrievals show increasing positive biases and decreasing percentages of retrievals falling within the EE envelopes as the elevation increases. By contrast, the DB retrievals are less affected by elevation changes with more than 76% of retrievals falling within the EE envelopes and small negative biases close to 0. Although the DTB retrievals are an improvement on the DT retrievals, they are still worse than the DB retrievals. This is because the DTB algorithm does not consider the effects of elevation changes in the merging procedure. Compared to the C6 DB retrievals, the C6.1 DB retrievals at high-attitude areas are greatly improved due to algorithm updates in artefact reduction and surface modeling for heterogeneous elevated terrains.

4.3.4. Uncertainty related to land cover type

For no or sparse vegetated areas (NDVI ≤ 0.2), the DT retrievals show large positive biases greater than 0.06 with less than 56% of retrievals falling within the EE envelopes (Fig. 9). The DB algorithm can provide ~6–12 times more retrievals and performs better with smaller

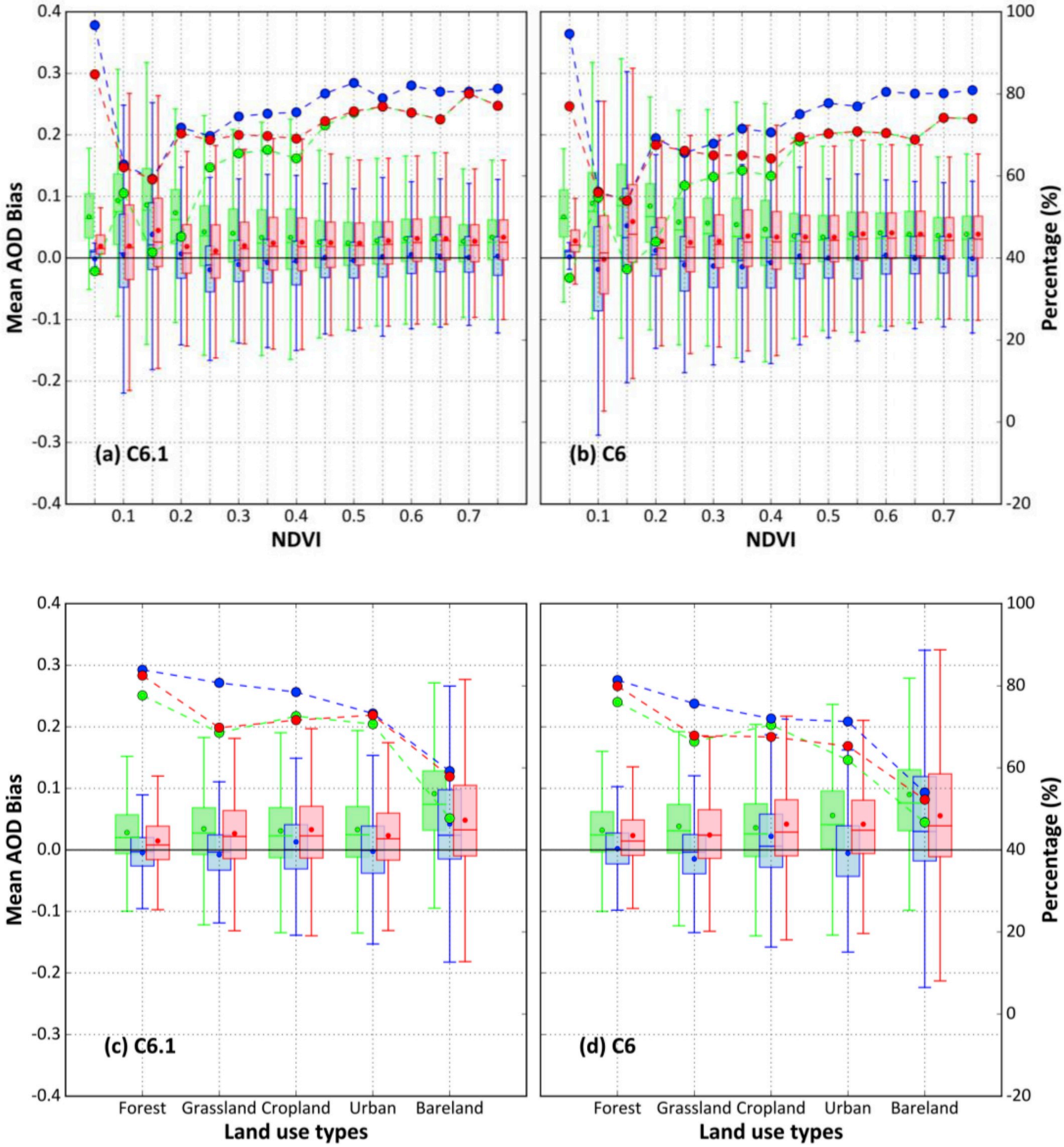

Fig. 9. Same as Fig. 6 but as a function of NDVI (a, b) and land use type (c, d).

biases, and more retrievals falling within the EE envelopes than the DT algorithm. The DTB and DB retrievals show similar performances because the merged product mostly adopts the DB values over such areas. For moderately vegetated surfaces (0.2 < NDVI < 0.5), the performance of DT algorithm improves, i.e., more retrievals falling within the EE envelopes and decreasing biases. The DB algorithm generates more retrievals with higher percentages of retrievals falling within the EE envelopes and smaller biases than the DT algorithm. The DTB retrievals are overall better than the DT retrievals but less reliable than the DB retrievals. For densely vegetated surfaces (NDVI ≥ 0.5), the DB algorithm performs the best with more than 72% of retrievals falling within the EE envelopes. The DTB and DT products show almost the same performances because the DTB product mostly adopts the DT values over these areas. The DTB retrievals are an improvement on the DT retrievals in low to moderately vegetated areas but overall worse than the DB retrievals in densely vegetated areas. This suggests that it is not always useful for the merging procedure only depending on the fixed NDVI thresholds. More appropriate approaches need to be explored.

Of the three vegetation types, the DT algorithm performs the best over forest but worst over grassland (Fig. 9). Meanwhile, the performance of C6.1 DT retrievals is much improved over urbans due to significant improvements in the estimation of surface reflectance compared to the C6 DT retrievals. However, it still shows large positive biases. The DT algorithm performs poorly over bare land with few successful retrievals and less than 48% of the retrievals falling within the EE envelopes, showing significant overestimations. The number of retrievals generated by the DB algorithm is greater than that generated by the DT algorithm for all land surface types, especially for the bare land and urban. The DB algorithm performs slightly better than the DT algorithm over forest and urban. Moreover, the DB retrievals are greatly improved than the DT retrievals over bare land, grassland and cropland. The DTB retrievals are similar in distributions with DT retrievals over grassland and cropland, yet with DB retrievals over bare land.

5. Summary and conclusions

Three aerosol optical depth (AOD) products, Dark Target (DT), Deep Blue (DB), and their merged (DTB), generated from MODIS in the newly released Collection 6.1 are cross-compared and validated over land and ocean in order to gain a knowledge of their accuracy and problems at global, regional and individual site scales. To gauge any improvement over the last release, the C6 AOD products were also employed for the same period (2013–2017). These satellite products are validated against ground-based AOD data from the new version (Version 3 Level 2.0) data derived from AERONET ground measurements observed at 384 sites.

There are no clear differences between the two collections over oceans, yet more noticeable differences are seen among the three aerosol datasets between the two collections over land, especially for the DB product. For example, significant positive differences are seen in Southeast Asia, the Middle East, northern South America, and central Africa, by contrast, the negative differences are found over Europe, northern Africa and central Asia. The DB retrievals are much lower than the DT retrievals over western North America, central Africa, East and South Asia. There is little difference between the DTB and DT retrievals over most land areas.

Regional validations show that the DT algorithm is more suitable for highly vegetated and low aerosol-loading areas in Europe and eastern North America. The DB algorithm performs better with higher fractions of the retrievals within the EE envelopes and lower estimation uncertainties than the DT algorithm in most selected regions. Although the DTB algorithm generates more retrievals, it does not beat the performance of the DB algorithm in many selected regions. Site-scale validations show that the DT algorithm performs the best at a few sites, by contrast, the DB algorithm shows the best performance in terms of almost all evaluation metrics at about half of the sites. The DTB and DT algorithms perform the best at 33% of the sites located in Europe, eastern North America, and Southeast Asia. In general, the C6.1 aerosol products are overall improved than C6 products from site, regional to global scales.

The uncertainty analysis shows that as the surface reflectance increases, the DT performance falls sharply, while that of the DB algorithm remains relatively stable. The DT (DB) algorithm performs poorly in continental- and dust-aerosol-dominated (strongly absorbing and dust-aerosol-dominated) areas. The quality of all aerosol datasets deteriorates as the aerosol loading increases, indicating that aerosol retrievals made under such conditions still face great challenges. The DB algorithm performs much better than the DT algorithm in high-elevation areas due to its artefact reduction and improved surface modeling over heterogeneous elevated terrains. The DT algorithm performs much more poorly than the DB algorithm over sparsely vegetated surfaces but improves as NDVI increases. For densely vegetated areas, the DB retrievals show similar good even better performance than the DT and DTB retrievals. Similar conclusions can be made when different land use types are considered. The comparison results illustrate that among the three aerosol datasets, DTB products are not always the best on site-specific to global scales. This suggests that it is not always right for the merging procedure only depending on the fixed NDVI thresholds, and more appropriate method considering various factors (i.e., land use, elevation, aerosol type) is needed and will be explored is our next work.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.atmosenv.2018.12.004.

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