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A total of eight years of Terra (2000–2007) and Aqua (2002–2009) Moderate Resolution Imaging Spectroradiometer (MODIS) Deep Blue (DB) collection 5.1 (c5.1) data were examined for their potential usage in aerosol assimilation. Uncertainties in the DB Aerosol Optical Depth (AOD) were identified and studied. Empirical corrections and quality assurance procedures were developed for North Africa and the Arabian Peninsula. After applying quality assurance and quality check procedures, the Root-Mean-Square-Error (RMSE) in the MODIS Terra and Aqua AOD are reduced by 18.1 and 18.2% to 0.16 and 0.17, respectively, with respect to AERONET data. These procedures were also applied to two months of DB collection 6 (c6) AOD data and reductions in RMSE were found, indicating that the algorithms developed for c5.1 data are applicable to c6 data to some extent. A new quality-assured DB level 3 AOD product was developed for future implementations in both aerosol data assimilation and climate related applications.

1 Introduction

Numerical weather prediction of aerosol phenomena has been implemented for air quality and visibility (Lelieveld et al., 2002; Park et al., 2003; Reid et al., 2004, 2009; Al-Saadi, et al., 2005; Hollingsworth et al., 2008). Recent studies have shown that satellite aerosol retrievals can be effectively used, through data assimilation, to improve accuracies of aerosol analysis and forecasts (e.g., Zhang et al., 2008, 2011; Benedetti et al., 2009; Sekiyama et al., 2010; Campbell et al., 2010). The operational MODIS Dark Target (DT) products in particular are attractive for assimilation, as they provide aerosol retrievals over global oceans and most land areas with near daily coverage. However, due to the high surface reflectance, traditional DT retrievals fail over bright surfaces such as the Saharan and Gobi deserts (Remer et al., 2005). This leaves large spatial gaps in the AOD record in desert regions, some of which host some

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of the largest aerosol loadings in the world. While other sensors such as the Multi Angle Imaging Spectroradiometer (MISR) and the Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observation (CALIPSO; Winker et al., 2009) can retrieve over bright surfaces, their limited swath and delayed data processing reduces efficacy in aerosol forecasting applications.

Because arid regions tend to have lower surface reflectance at shorter wavelengths, traditional DT method can often be successfully applied in blue wavelengths. The Deep Blue algorithm takes advantage of this surface phenomenology, performing aerosol retrievals at blue wavelengths (such as the 0.47 μm spectral channel in MODIS) and utilizing the selected aerosol model in the inversion to generate AOD (Hsu et al., 2004, 2006). The DB algorithm has been successfully applied to both MODIS instruments and SeaWiFS to allow for large swath coverage for aerosol retrievals over and around desert regions. DB has shown that aerosol optical properties can be retrieved with tolerable uncertainties, even over deserts and semi-arid regions, where traditional DT methods applied to mid visible and red wavelengths have difficulties (Shi et al., 2011b; Li et al., 2012). This has allowed DB to be applied to such sensitive applications as source function development (e.g., Ginoux et al., 2010).

While filling a significant data gap, the use of DB specifically in data assimilation applications requires the development of a prognostic error model. That is, an uncertainty needs to be assigned to every retrieval. Such errors are not commonly reported by aerosol retrieval developers. Instead, bulk global uncertainties are given, often expressed as an error range and a fraction of retrievals falling within that range (e.g., MODIS Dark Target – DT – over-land AOD has an expected error range of $\pm 0.05 \pm 0.15 \times \text{AOD}$, and roughly two-thirds of MODIS DT collection 5.1 – c5.1 – AOD fall within that error range, Levy et al., 2005). Given that uncertainty is well known to be related to spatially correlated features such as land surface albedo and aerosol microphysical properties, the use of a single uncertainty value can result in large errors in models during assimilation. The inclusion of data from a region with poorly constrained lower boundary conditions could, for example, result in a fictitious “aerosol

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simulation to generate lookup tables (LUTs) describing the observed satellite radiance at 0.412, 0.47, and 0.65 μm as a function of AOD at 0.55 μm , aerosol type, and surface albedo. Using a maximum likelihood method, the optimal combination of aerosol models is selected by matching the observed radiance to the LUT values. For pure dust aerosol cases, AOD and single scattering albedo are reported at 0.412 and 0.47 μm , while for mixed aerosol cases, AOD and Angström Exponent are reported (Hsu et al., 2004). The DB data include a Quality Assurance (QA) flag that labels the data into three categories: “none”, “good”, and “very good”. The DB data also include other ancillary parameters such as viewing/scattering angles, solar zenith/azimuth angles, surface albedo, and number of pixels used, all of which were used in this study for evaluation purpose.

MODIS c5.1 DB data are currently available for 2002–2010 from Aqua, and 2000–2007 from Terra. The spatial coverage of the data includes North Africa, the Arabian Peninsula, part of Central Asia, India, Australia, the Western US, and Andes Mountains. The spatial resolution of the data is 10 km at nadir and the revisit time is about one to two days. Compared to MISR, which also retrieves aerosol properties over bright surfaces, DB has a much wider spatial coverage and a more frequent revisiting time. The uncertainties of DB AOD retrievals are listed as 20–30 % of the AERONET AOD values (Hsu et al., 2008).

This study is based on the comparisons of MODIS DB c5.1 and AERONET AOD, coupled with a contextual analysis of retrieved aerosol features. The quality assured level 2.0 Aerosol Robotic Network (AERONET) AOD data with a stated uncertainty of 0.015 were used as the “ground truth” (Holben et al., 1998). Eight years of AERONET AOD data were collocated in space and time with Aqua DB (2002–2009) and Terra DB (2000–2007), following the method mentioned in Shi et al. (2011a). Using this method, a pair of DB and AERONET AOD data samples is considered collocated if the temporal difference between the two data samples is within ± 30 min, and the spatial distance is within 0.3° (latitude/longitude). Note that, since the 0.55 μm is the primary wavelength used for data assimilation, only DB AOD data at this wavelength were used in



this study. However, no AERONET data are available at this spectral channel. Therefore, AERONET data from the 0.50 and 0.67 μm spectral channels were interpolated to derive AOD values at the 0.55 μm channel following O'Neill et al. (2003).

3 Evaluations

In this section, the general performance of DB is described, along with the sources of uncertainties in the DB products with respect to observing conditions, and Quality Assurance (QA) flags provided by the DB products. Details of the evaluation procedures are illustrated in Table 1. Tests performed include analyses for boundary conditions, viewing geometry, cloud contamination, aerosol microphysical properties, and other observing conditions. All analyses were conducted for both Terra and Aqua DB products, however, in most cases, only analyses from Aqua DB data are shown, as similar structures are found for the Terra DB product. The analyses for the Terra DB product are provided in the supplemental materials unless specifically mentioned.

3.1 Overall nature of the Deep Blue product

This section starts with the simple global evaluation of the DB product, and then describes the selection of areas with sufficient collocated AERONET and DB data for further evaluation. Figure 1 shows the global comparisons of the collocated Aqua DB and AERONET AOD with respect to different QA flag settings. This figure displays the traditional method of evaluating satellite data against AERONET, which is used to diagnose the uncertainties in the data set. The regression equation $\tau_{\text{DB}} = b + a \cdot \tau_{\text{AERONET}}$ is diagnostic and describes the quality of the retrieval against a more accurate reference dataset (in our case, AERONET AOD, τ_{AERONET}). By contrast, the regression equation $\tau_{\text{AERONET}} = b + a \cdot \tau_{\text{DB}}$ is prognostic and describes the linear transformation that will produce values that are closest to the reference data. In this study, diagnostic regression

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is used to capture data characteristics, and prognostic regressions are used to develop correction factors and uncertainty estimation models.

This study makes extensive use of root mean square errors (RMSE), which are calculated using Eq. (1)

$$5 \quad \text{RMSE} = \sqrt{\frac{1}{n} \sum_n (\text{AOD}_{\text{AERONET}} - \text{AOD}_{\text{DB}})^2} \quad (1)$$

and represent the bias of the evaluated data sets towards the ground truth. The uncertainty estimation model, following Zhang and Reid (2006), is based on a prognostic equation to estimate RMSE as a function of DB AOD. Development of this uncertainty estimate is discussed in Sect. 5.

As Fig. 1 shows, DB AOD values have a RMSE of 0.234 with respect to AERONET AOD globally, an r^2 value of 0.81, and a slope of 0.87 for all available data. A total of 42.8 % (14 023) of DB AOD data points fell outside the reported uncertainty range, defined by $\pm 0.05 \pm 20\% \times \tau_{\text{AERONET}}$ (Huang et al., 2008). When only data with a QA of “very good” are used, the RMSE drops to 0.207, r^2 increases to 0.86, the slope changes to 0.83, and the fraction of outliers drops to 31.7 % (1038). Although the regression slopes in Fig. 1 are not dependent on QA flags, the 11.5 % decrement in RMSE and 11.1 % decrement in outliers from QA flags equal to “none” to “very good” show that higher quality data are selected when using the “very good” QA flag. However, in addition to an improved performance, an 84.3 % data loss is found.

The performance of the DB AOD retrievals, however, shows a regional dependence, particularly in regard to slope. This is suggestive of microphysical bias. Using all available data with the “very good” QA flag, regional comparisons between Aqua DB and AERONET for nine selected regions were conducted as shown in Fig. 2, with Fig. 3 showing the domain of each area in a different color. As indicated from Fig. 2, only four regions, namely North Africa, Europe, East Asia, and West Asia, have more than 400 collocated data points. The remaining regions, Western North America, Eastern North America, South America, South Africa, and Australia, have insufficient numbers

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of collocated Aqua MODIS and AERONET data points. Of the nine selected regions, the best performance of the DB data is found over North Africa, with a slope of 1.16, an r^2 value of 0.81, and an AOD RMSE of 0.19 between DB and AERONET AOD. However, high bias occurs when AOD is greater than one, which could be caused by multiple scattering. Contrary to the overestimation of AOD values over the North Africa region, an underestimation of AOD values is found for DB retrievals over Asia, with a much higher RMSE of 0.213 for West Asia and 0.286 for East Asia. Regions other than North Africa either have very few collocated DB and AERONET data points, or have a much larger scatter between satellite and AERONET AOD values. The diagnostic and prognostic RMSE models were built for regions in Fig. 2 with more than 400 data points, namely Europe, North Africa, East Asia and West Asia (Fig. 4a, b). Europe, shown in black in Fig. 4a, b, has low RMSE at low AERONET AOD, but higher RMSE at low DB AOD. This can be explained if DB is systematically underestimating AOD in this region, a possibility we will examine later in this section. Because of limited data volume and range of retrieved AOD in the matched datasets, only the North Africa and Arabian Peninsula regions (namely “the study region” from now on) were used to construct the DA-quality DB products. These regions will be the main focus of discussion in this paper.

Focusing on the study region, the diagnostic RMSE analysis as a function of AERONET AOD was performed for all data and data with QA flag values of “good” and “very good” (Fig. 4c, d). For all available data and data with “good” QA flags, the RMSE values from Aqua and Terra are very similar in both magnitude and pattern. When AERONET AOD values are smaller than 0.8, the RMSE values from both sensors remain relatively constant. Above this value, the RMSE increases as AERONET AOD increases. With a strict QA flag filtering, the RMSE values of DB AOD reduce to approximately 0.1 for AERONET AOD below about 0.4, with a larger reduction of RMSE shown in Aqua data.

Shown in Figs. 1 and 2, the QA flag is necessary for highlighting retrievals that are the most “trustworthy” (Hsu et al., 2004). However, there are limitations in using data

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with only “very good” QA flags. For example, using the QA flag also introduces artifacts in AOD spatial distribution. Figure 5 shows the daily spatial distribution of DB AOD over the study region for 1, 2, and 3 May 2006, with all available data on the left panel, and data with only QA flags of “very good” on the right panel. For all three days, two patterns can be observed consistently for figures from the right panel: (1) retrievals in the center of the swaths are removed which are due to the large scattering angles; (2) the number of retrievals is largely reduced south of 13° N, and a significant portion of low AOD retrievals are excluded by the “very good” QA flags. When averaged over a one-year period (Fig. 6), the second pattern shows up as a near-linear feature, indicated by much higher AOD values for “very good” data below 13° N (Fig. 6a, b). This pattern is introduced by a significant reduction in the number of retrievals, especially low AOD retrievals as shown in Fig. 5, when applying the “very good” QA filters (Fig. 6c). This reduction in data samples was caused by artificial thresholds in the DB retrieval algorithm, considering the number of pixels used in the retrieving process. Despite the disadvantage of applying “very good” QA flags, only DB data with the “very good” QA flags were used hereafter, because of reduced error in these data, and because of systematic bias in AOD values with other QA flags (see Sect. 3.2.1).

3.2 Detailed analysis for DB over North Africa and Southwest Asia

Series of analyses were performed to investigate the sources of uncertainty in DB AOD product, including angular dependence, aerosol microphysics, surface reflectance, and other observing conditions. “very good” quality data were used to conduct most of the analyses except that of angular influences, due to the change of behaviors between all available data and data with “very good” quality. Although most discussions are focus on the study region only, global analysis is performed for the aerosol microphysics studies (Sect. 3.2.2), as insufficient numbers of fine mode aerosol retrievals are available at the study region.

3.2.1 Angular dependence

An interesting discrepancy between the DB AOD with and without QA flag filtering was discovered for angular dependency in AOD bias. For data with QA flag equals to “very good”, no systematic bias (AERONET AOD minus DB AOD, symbol as $\Delta\tau_{A-M}$) is found as functions of viewing zenith angle (θ). However, with all data, there is a strong relation between increasing viewing zenith angle and increasing $\Delta\tau_{A-M}$. Figure 7 shows the average difference between DB and AERONET AOD (ΔAOD) at $0.55 \mu\text{m}$ as a function of θ over the study region. A decreasing trend in $\Delta\tau_{A-M}$ is found as θ values increase for the raw DB data. The $\Delta\tau_{A-M}$ values are around -0.09 for θ values ranging from 0° to 10° , and are almost zero when θ values exceed 50° . However, this relationship between $\Delta\tau_{A-M}$ and θ is non-existent when the “very good” QA flag filtering is applied (Fig. 7b). Similar patterns were found for scattering angle, but not shown in this paper. The influence of the viewing angle was then decoupled with albedo at $0.412 \mu\text{m}$. It is shown that, when the surface is relatively bright (albedo between 5 and 11 %), the influence from the viewing angle is minimized. When the surface is dark (albedo smaller than 5 %), the bias of AOD varies with viewing angle for all available data.

3.2.2 Aerosol microphysics

Four aerosol microphysical parameters were evaluated for their impacts to the retrieval bias under cloud free conditions. The four parameters were Angström Exponent and Single Scattering Albedo (ω) from the DB product, fine mode fraction (η) calculated from AERONET data using a spectral convoluted method from O’Neil et al. (2001), and the aerosol type flag included in the DB QA flag. Among all the parameters, investigations showed that the DB AOD errors are most sensitive to η . Only one third of the aerosol retrievals over the study region have $\eta > 0.5$ and all of which are smaller than 1.0. Also, all data from the matched dataset with $\eta < 0.5$ are from the study region. Figure 8 shows the scatter plot of DB vs. AERONET AOD for two η ranges: $\eta < 0.5$ (Fig. 8a) and $\eta > 0.5$ (Fig. 8b). Underestimation of AOD is found for coarse particles

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with $\eta < 0.5$, and an overestimation is found for fine particles with $\eta > 0.5$ globally. Consistent relationships are also found over the study region. Since nearly two-thirds of DB aerosol retrievals in the matched dataset over the study region have $\eta < 0.5$, it is likely that AOD over the study region as a whole is underestimated by DB.

Although convincing trends are found with respect to η , a parameter that is included in the DB products needs to be selected and used for empirical corrections mentioned in a later section. Thus, other microphysical parameters, including Angström Exponent and ω , were also examined, site by site, and seasonally. However, no significant trends are found for these two parameters. A comparison was made between the retrieved Angström Exponent and AERONET derived η , no relation between the two parameters was found. At last, the aerosol type flag, a parameter that is included in the DB products, was used to represent the aerosol microphysics in the empirical correction steps (see Sect. 4).

3.2.3 Surface reflectance

The DB algorithm is built based on a theory that bright surfaces look relatively dark at the blue wavelengths (Hsu et al., 2004). Therefore, it is necessary to evaluate the influence of albedo on AOD retrievals. Also, as mentioned in Sect. 3.2.2, Δ AOD can be affected by inaccurate assumptions of aerosol microphysical properties in the retrieval process. To decouple the effects of aerosol microphysics and surface albedo on Δ AOD, the surface albedo related DB AOD bias was investigated as a function of aerosol type and fine/coarse aerosol modes. Again, global data were used to observe the fine mode aerosol performances and the coarse mode particle analyses are the same for the study region.

For all analyses, the collocated DB and AERONET AOD data were separated into four groups based on DB surface albedo (α) at a wavelength of $0.412\mu\text{m}$. The four albedo ranges are 0–5 %, 5–8 %, 8–11 % and above 11 %. Figure 9 shows the spatial distribution of the selected albedo ranges over the study area. Illustrated in Fig. 9, areas with albedo values higher than 11 % are located over the white sand deserts,

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and regions with albedo values lower than 5 % are located over semi-vegetated areas. The influences of surface albedo as well as η to DB AOD data are shown in Fig. 10. Here again, all collocated DB and AERONET data are included as there are insufficient fine mode AOD retrievals over the study area. Left panels of Fig. 10 show that for $\eta < 0.5$ (coarse mode), when α is less than 11 %, an underestimation in satellite AOD is observed, and a strong non-linear trend is found. The magnitude of the underestimation is reduced when α increases from 5 % to 11 %. For $\eta > 0.5$ (fine mode), however, an overestimation is found for low albedo ranges, but not for the 8–11 % albedo range (Fig. 10, right panels). In general, for coarse mode aerosols, a higher albedo results in a smaller underestimation, and for fine mode aerosols, an opposite pattern is observed. Also illustrated in Fig. 10, large scatter is found between DB and AERONET AOD when surface albedo (0.412 μm) values are greater than 11 % for both $\eta > 0.5$ (fine mode) and $\eta < 0.5$ (coarse mode) cases. Figure 10 highlights the necessity of decoupling the surface and aerosol microphysical factors for empirical corrections.

3.2.4 Observing conditions

Cloud contamination is one of the potential sources of uncertainties for satellite aerosol products. However, 93 % of retrievals with “very good” QA are free of MODIS-detected cloud. The error statistics of the remaining 7 % do not show significant differences, and do not demonstrate the systematic offset in AOD shown in the MODIS dark-target over-land product (Hyer et al., 2011).

DB products also contain a parameter that records the number of 1-km pixels used in creating the 10 km resolution AOD retrievals. The quality of the DB retrievals was checked with respect to this parameter, and a noticeable high bias in $\Delta\tau_{A-M}$ of 0.05 was found if fewer than 20 1-km pixels are used in the retrieval process, as shown in Fig. 11. No significant bias was found for retrievals with more than 20 1-km pixels used in the retrieval process. This pattern of increment in $\Delta\tau_{A-M}$ when number of pixels used is less than 20 is not found in Terra (see Supplement Fig. 6).

3.3 Statistical analysis for spatial variations

In Sect. 3.2, sources of physical-based uncertainties of the DB AOD have been identified. The DB aerosol data are reported at a spatial resolution of 10 km, and, therefore, the regional variations of surface albedo and aerosol optical properties within the 10 km domain could also affect the accuracy of the DB AOD values, as illustrated by Eq. (2). Equation (2) shows the relationship between the uncertainties in DB AOD values and three main contributors: (1) regional variations of AOD (STE_{AOD}), (2) regional variations of surface albedo (STE_{sfc}), (3) physical based uncertainties as described in Sect. 3 (physical parameters, or PP).

$$\Delta AOD = \frac{\partial AOD}{\partial STE_{sfc}} dSTE_{sfc} + \frac{\partial AOD}{\partial STE_{AOD}} dSTE_{AOD} + \frac{\partial AOD}{\partial PP} dPP \quad (2)$$

Here, STE_x represents the spatial variance of parameter x and is defined as the standard error of component x that is calculated using:

$$STE = \frac{\sigma}{\sqrt{N}} \quad (3)$$

where

$$\sigma = \sqrt{\frac{1}{N} \sum_{i=1}^N (x_i - \mu)^2} \quad (4)$$

N is sample size, x_i is each sample value, μ is the expected value, and σ is standard deviation. The standard error is calculated using a 3×3 (approximately 30 km \times 30 km) moving window around a given aerosol retrieval.

The goal of this study is to evaluate potential sources of uncertainties in the DB aerosol products, and to develop quality assurance steps and empirical methods to minimize bias and noise. Therefore, the first two terms from the right hand side (RHS)

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of Eq. (2) need to be studied and removed for the further development of empirical correction methods. It is difficult to completely decouple the three terms listed in the RHS of Eq. (2). However, it is possible to identify scenarios that minimize the first two terms, as shown in Fig. 12.

Figure 12 shows the analyses of normalized ΔAOD ($\Delta\tau_{A-M}$ over DB AOD) as a function of STE_{sfc} with respect to surface reflectance (Fig. 12a), DB AOD (Fig. 12b), and aerosol type (Fig. 12c). Figure 12a shows that for darker surfaces (albedo smaller than 8%), the variation of SDE_{sfc} is low. Higher SDE_{sfc} values are found over regions with brighter surfaces (e.g., 8% < albedo < 11%), especially when normalized aerosol bias becomes negative. Figure 12b suggests that larger STE_{sfc} values correspond to regions with low AOD values. When normalized aerosol bias reaches -1.0 , the largest mean values of STE_{sfc} correspond to AOD values smaller than 0.25. When separating the STE_{sfc} based on aerosol type, the STE_{sfc} of smoke particles oscillates around 0.0015, while those of “mixed” and “dust” particles fluctuate at much larger values and reach 0.003. This indicates both “mixed” and “dust” aerosol retrievals contain data that are largely biased by STE_{sfc} . The next section describes how scenarios with significant contributions from from STE_{sfc} and STE_{AOD} were identified and removed as part of the QC procedures.

4 Development of QA/QC procedures for DA-quality DB over North Africa and Southwest Asia

Based on discussions from Sect. 3, Level 3 DA-quality DB data over the study region were constructed in two steps. Initially, noisy data were removed using various filters, including QA flags, standard error check, and buddy checks over the study region. Table 2 shows all the filtering standards with corresponding data loss. Next, empirical corrections were applied based on each of the aerosol microphysical properties and surface conditions.

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5 Estimation of prognostic uncertainty for DA-quality DB AOD

Using the data screening steps and empirical correction procedures mentioned in the previous section, the DA-quality DB AOD data were generated. In this section, the accuracy of the newly generated data was evaluated through inter-comparison with ground observations and through the prognostic and diagnostic models of the RMSE.

The comparison of DB and AERONET AOD before and after the quality assurance and empirical corrections steps are shown in Fig. 17 for Aqua and Terra over the study region in order to estimate the prognostic uncertainty. Reductions in both bias and noise are clearly visible for both DA-quality Terra and Aqua DB AOD data. The slopes of AERONET and the newly generated DB AOD are close to 1 in prognostic comparisons for Aqua (0.99) and Terra (1.03) MODIS. The non-linear features for both Aqua and Terra are weakened, but not eliminated, due to the restriction in empirical corrections that the multipliers cannot exceed 1.3. The RMSE values were checked for three AOD ranges: total AOD, AOD greater than 0.5 and AOD greater than 1.0. The corresponding RMSE are from 0.19 to 0.16 with 18.1 % error reduction, from 0.33 to 0.24 with 26.3 % reduction, and from 0.54 to 0.37 with 32.3 % reduction for Aqua (Terra) after applying the QA steps and empirical corrections. Similarly for Terra, the corresponding RMSE are from 0.24 to 0.17 with 18.2 % error reduction, from 0.35 to 0.27 with 22.9 % reduction, and from 0.55 to 0.35 with 36.4 % error reduction. The total data losses, calculated against the total number of retrievals with “very good” QA flags, are 28.5 % for Aqua and 44.5 % for Terra.

Figure 18 shows the RMSE of the new product as a function of DB AOD before and after all processes. The upper panels are for total AOD, while the lower panels are separate dust and mixed aerosol types. Smoke aerosol particles were not included due to insufficient data samples. As Fig. 18a, c shows, RMSE values are reduced for all AOD ranges after the correction processes. For total AOD less than 0.4, the noise floors of RMSE of original and newly generated data are 0.113 and 0.104, respectively. Different trends are found for different aerosol types. For example, the RMSE values

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show an increasing pattern as DB AOD increases for mixed-type aerosol particles. However, for dust particles, the minimum RMSE appears around DB AOD value of 0.3. This V-shaped RMSE distribution indicates a larger retrieval uncertainty for dust AOD values smaller than 0.3. Figure 18b, d shows a similar analysis to Fig. 18a and c, but use Terra DB data. One distinct difference from Fig. 18a and c is that no noise floor of RMSE is found. In the prognostic analyses, a sudden increase of RMSE values is found at an AOD value around 0.5. This sudden increase in RMSE values is due to outliers from the mixed type of aerosol particles under high surface albedo case (see Fig. 8 of the Supplement for details). Other than this instance, generally, the RMSE analyses show that the newly generated DA-quality data has smaller RMSE values when compared to the original data.

The level 3 quality-assured data were generated over the study region by spatially averaging the AOD data in a quarter-degree latitude and longitude resolution. Figure 19 shows the spatial plots of the original DB data, the “very good” QA quality DB data, and the newly generated data for Terra and Aqua separately for 2007. The main features are similar before and after the empirical corrections and QA procedures. When compared with DB data that has the “very good” QA flag, high AOD noise was reduced, and general AOD values were increased due to the correction of the non-linear features. All data with surface albedo values exceeding 11 % were removed. Also, data for regions below 13° N were not included due to the QA-filtering issue mentioned in Sect. 3.1. It is shown in Fig. 19 that Terra AOD have higher values, approximately 0.1, than Aqua AOD. Knowing that dust aerosols have a diurnal feature, the difference in local passing time for the two satellites may cause this problem. Also Terra AOD have a larger bias, as shown in Figs. 4d and 18b, which can also contribute to this problem.

As an independent study, we have also evaluated the newly generated level 3 Aqua DB AOD data for 2010 and 2011 that are not included in the analyses as mentioned in sections 2–4. AERONET level 1.5 data were used instead of AERONET level 2.0 data, since level 2.0 AERONET data were not available from all sites over the study region for 2010 and 2011 when the study was conducted. Again, with the empirical correction

and quality assurance steps, both bias and noise are reduced. The RMSE for newly generated data is reduced 11 % from 0.227 to 0.202, and the r^2 changes from 0.74 to 0.77 for prognostic purpose (Fig. 20). Noted that there were four outliers that showed in blue dots from Fig. 20, which were manually removed from the analyses for both original and DA-quality DB data.

6 Preliminary analysis using the collection 6 MODIS DB data

A new version of the MODIS DB product (collection 6, c6) is currently under development with a targeted release date of next year. C6 of the DB algorithm includes important updates to the retrieval process and the QA flag standards, resulting in important differences in the data product, including a large increase (roughly 2x) in the number of retrievals with “very good” QA flags. We therefore, tested the algorithm developed in this study using two months (April 2006 and July, 008) of preliminary c6 DB data. Applying the empirical corrections and QA procedures that were developed based on DB c5.1 data to DB c6 data with QA equal to “very good”, the modified DB c6 data had a reduced RMSE, from 0.160 (preliminary DB c6) to 0.137 (Modified DB c6) for total AOD and from 0.11 to 0.07 for AOD greater than 0.5 (Fig. 21), using AERONET AOD as truth. The slope of the comparison between DB c6 and AERONET AOD also became closer to one, increasing from 0.79 to 0.94. Similarly, a higher r^2 value of 0.809 was found, compared to 0.688 for the preliminary DB c6 data. This preliminary analysis indicates that issues identified and quality assurance steps developed from this study are partially applicable to the DB c6 data.

Quarter by quarter degree averaged AOD spatial distributions of DB c6 data were also plotted for April 2006 and compared to the DB c5.1 data distributions. Figure 22 includes an AOD monthly map over the study region for all available data, “very good” QA data, and DA-quality data for both c5.1 (left panels) and c6 (right panels). Several significant changes between the spatial distributions were observed. One significant change is that the AOD pattern in DB c6 data is smoother for all three categories of

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coarse mode aerosols, the higher the surface albedo is, the lower the underestimation of DB AOD. For fine mode aerosols, however, the higher the albedo is, the lower the overestimation of DB AOD.

3. The new QA and empirical correction procedures were constructed, and new level 3 DB c5.1 products were created for future implication in data assimilation. Reductions in RMSE, which were calculated using ground-based AOD from AERONET as truth, of 18.1 and 18.2%, were found for the quality-assured products when compared to the original DB products for Aqua and Terra DB products, respectively.
4. An independent validation of DB c5.1 data over 2010 and 2011 was also conducted and improvements to the new data set were found as well. The newly developed level 3 products will be used in aerosol data assimilation and aerosol climate studies.
5. Lastly, the algorithm developed from this study was also tested using the preliminary DB c6 data that is targeted to be released next year. The quality assurance steps developed from the DB data c5.1 improve the accuracy of DB c6 data indicating that the algorithm and methods developed from this study can at least, partially applicable to the new version DB data. Also, we are hoping that issues identified from this study can provide useful information to the DB team in developing the up-coming DB data.

Supplementary material related to this article is available online at:
<http://www.atmos-meas-tech-discuss.net/5/7815/2012/amtd-5-7815-2012-supplement.pdf>.

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Acknowledgement. This research was funded by the Office of Naval Research Code 322 and the NASA Interdisciplinary Science Program. Yingxi Shi is funded by the NASA Earth and Space Science Fellowship Program. We acknowledge and appreciate the AERONET program and their contributing principal investigators and their staff for establishing and maintaining the coastal sites used in this investigation. We also appreciate MODIS DeepBlue team provide us the preliminary MODIS DB c6 data.

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Table 1. Flow chart of producing level 3 DB DA quality aerosol product.

Step 1	Step 2		Step 3	Step 4		Step 5
QA check	Analyses		Standard Error Check (STE _x)	Empirical Corrections		Aggregate to level 3 data
QA = very good	Considered Parameters	Albedo (α)	Standard error of AOD (τ) (STD _{AOD})	Using the regression relations found in Step 2 to correct DB AOD	α	Pixel level DA-quality data were averaged into 6 hourly one degree resolution data for model use
		Decoupled α with fine mode fraction (η)				
		Decoupled α with Aerosol type				
		Angström Exponent	Decoupled STD _{sfc} and STD _{AOD}		Decoupled α with Aerosol type	
		Single scattering albedo (ω)				
		Cloud Fraction ($F_{\text{cl,d}}$)				
		Viewing Angle				
				Cloud Fraction ($F_{\text{cl,d}}$)		

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Table 2. Filters and thresholds that are used in QA procedures with corresponding data loss for generating DA-quality Aqua DB AOD product, with data concerning Terra DB were presented in prentices. The percentage of data loss for all procedures after the QA filtering were calculated based on the data number that had QA equal to “very good”.

	QA Flag	Standard error of AOD (STD_{AOD})	Decoupled STD_{sfc} and STD_{AOD}	Cloud fraction (F_{cld})
Thresholds	“very good”	$STD_{AOD} >$ values in Eq. (6) (5)	$STE_{sfc} < 0.004$ and $STE_{AOD} < 0.03$	$F_{cld} < 60\%$
Data loss	84.3 % (82.6 %)	7.0 % (10.9 %)	20.8 % (33.1 %)	0.7 % (0.5 %)

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Table 3. Coefficients that used in the empirical corrections for Aqua DB data.

Aerosol type	Parameters	Range of surface albedo (α) at 0.412 μm		
		0.0–0.05	0.05–0.08	0.08–0.11
Mixed	offset	0.00697 (0.0; AOD < 0.25)	–0.0134	0.0
	slope	1.201 (0.887; AOD < 0.25)	1.149	1.0
Dust	offset	0.0	0.0 (0.0; AOD < 1.0)	–0.0285
	slope	1.3	1.3 (1.0; AOD < 1.0)	1.038
Smoke	offset	0.0		No data were taken in this range
	slope	1.3		

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Table 4. Coefficients that used in the empirical corrections for Terra DB data.

Aerosol type	Parameters	Range of surface albedo (α) at 0.412 μm		
		0.0–0.05	0.05–0.08	0.08–0.11
Mixed	offset	–0.0107	0.0261	No change
	slope	1.264	1.056	
Dust	offset	0.0	0.0 (0.0869; AOD < 0.9)	–0.0502
	slope	1.3	1.3 (0.705; AOD < 0.9)	1.145
Smoke	offset		0.0	No data were taken in this range
	slope		1.3	

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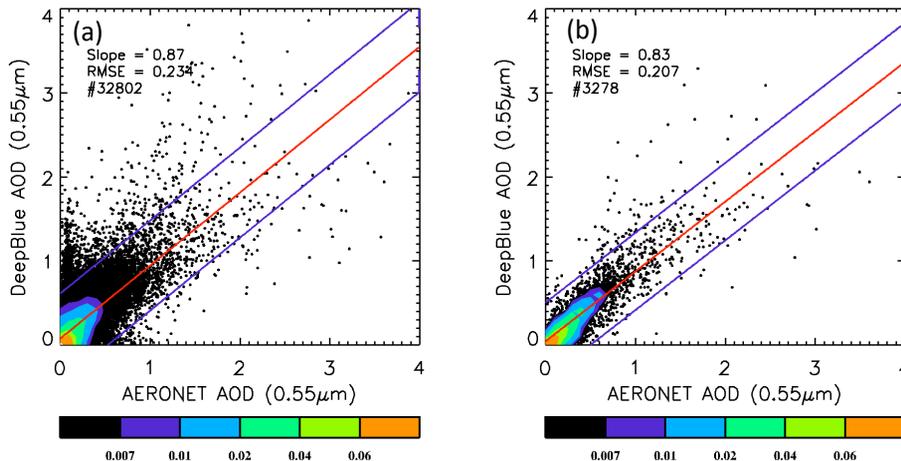


Fig. 1. Comparisons between Aqua DB and AERONET 2002–2009 for diagnostic purpose for (a) all data, (b) data with very good QA quality globally. The red line is the linear fit line and the blue lines are the 95 % confident interval lines. The color contour showed the percentage data density.

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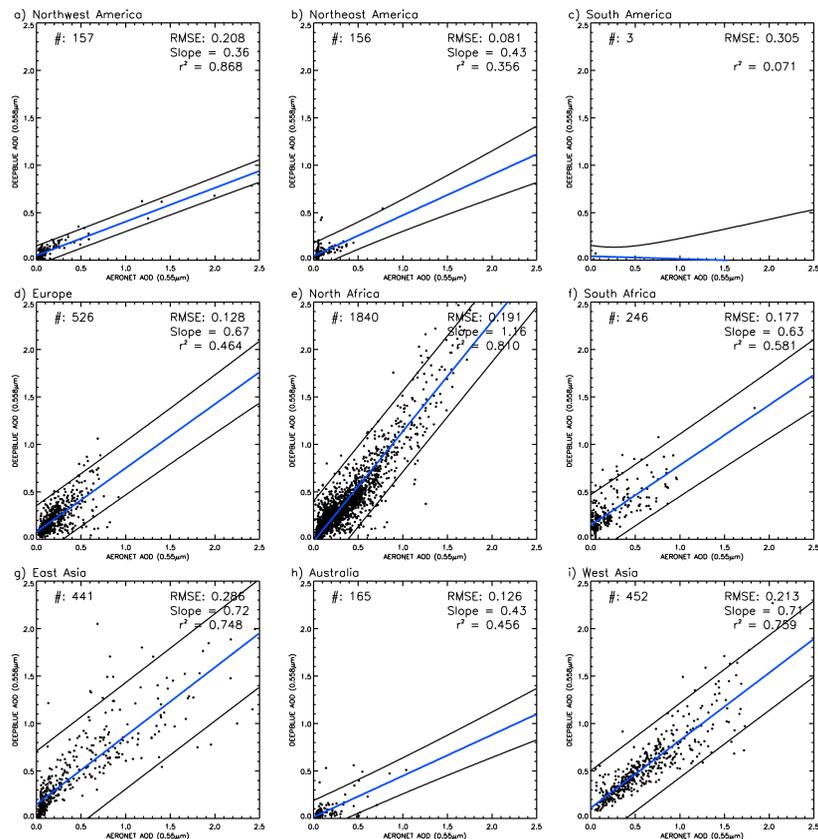


Fig. 2. Regional comparisons between Aqua DB AOD and AERONET AOD 2002–2009 with only QA equals to “very good” for **(a)** Northwest America, **(b)** Northeast America, **(c)** South America, **(d)** Europe, **(e)** North Africa, **(f)** South Africa, **(g)** East Asia, **(h)** Australia, and **(i)** West Asia. The blue line is the linear fit line and the black line is the 95 % confident interval line.

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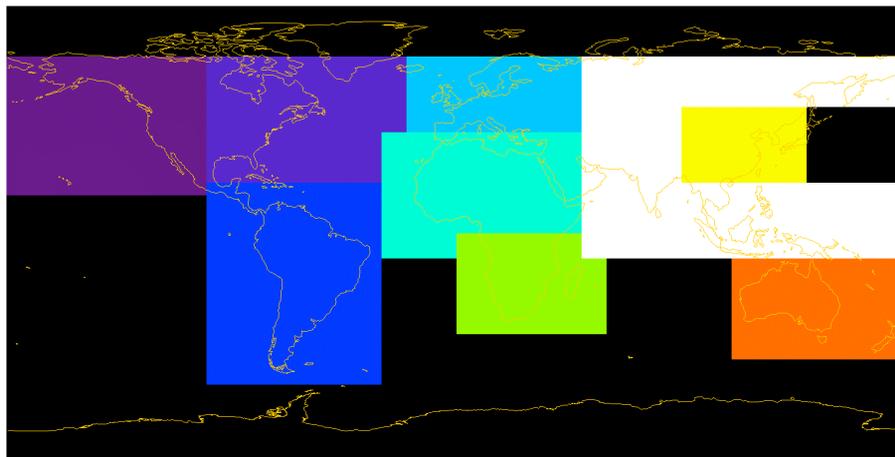


Fig. 3. The domains for areas that are shown in Fig. 2. Western North America is shown in indigo, Eastern North America is shown in dark slate blue, South America is shown in blue, Europe is shown in sky blue, North Africa is shown in spring green, South Africa is shown in lemon green, Australia is shown in orange, West Asia is shown in white, East Asia is shown in yellow, and other region is shown in black.

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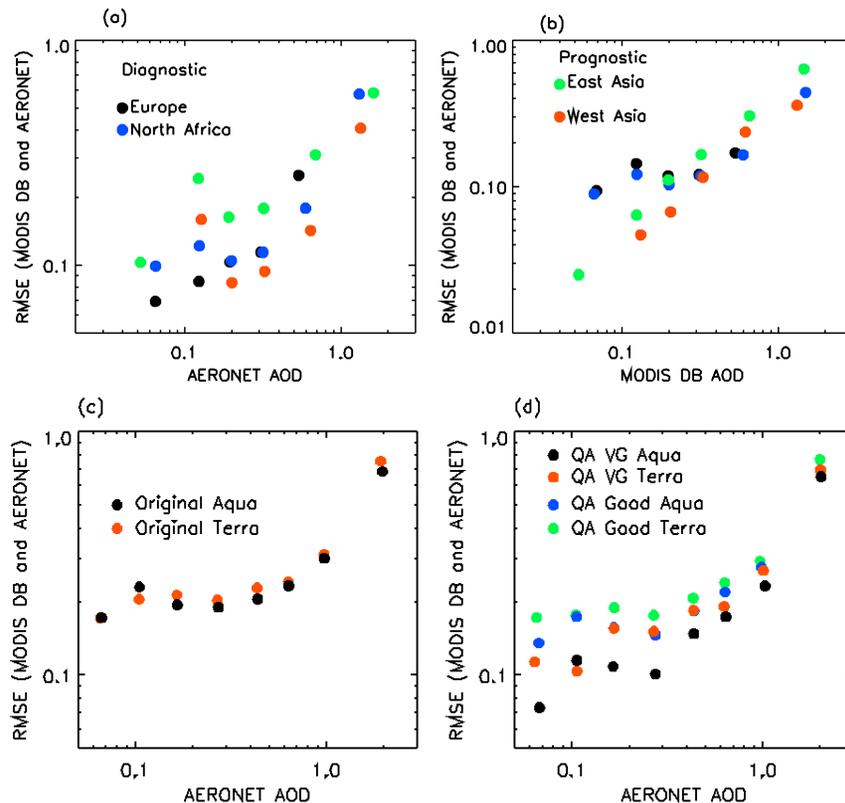


Fig. 4. The RMSE of DB AOD against AERONET AOD for **(a)** data with “very good” QA flag over Europe (black), North Africa (blue), East Asia (green), and West Asia (red) in Fig. 2 as a function of AERONET AOD, **(b)** similar as **(a)** but as a function of DB AOD, **(c)** all data over North Africa as a function of AERONET AOD and **(d)** similar as **(c)** but with data with QA equals to “very good” and “good”.

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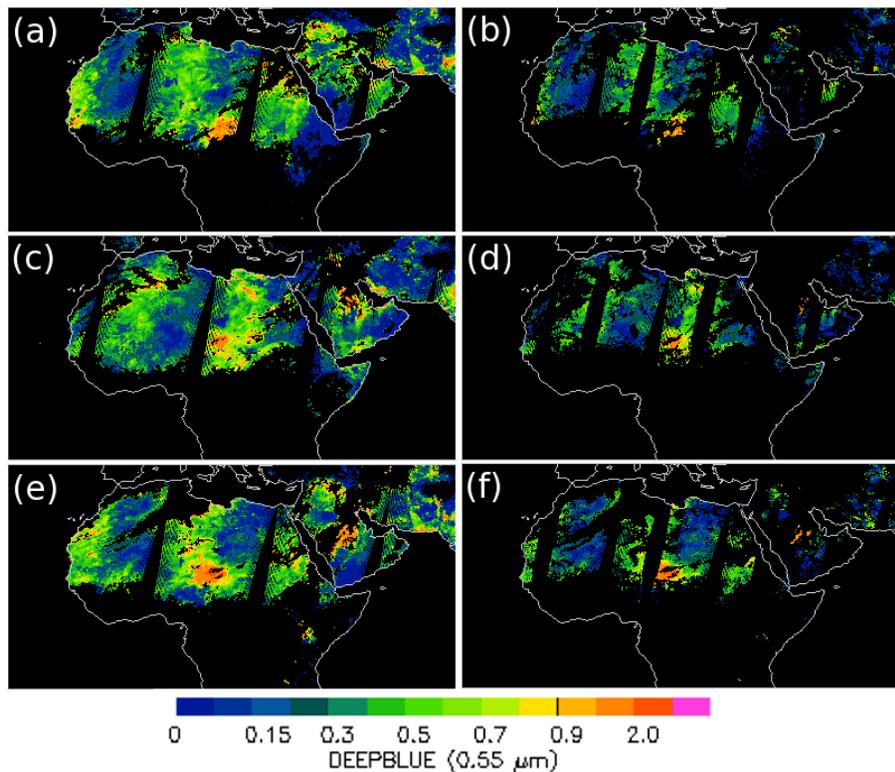


Fig. 5. Quarter degree spatial average of satellite aerosol observation over studied region for DB AOD for three days for **(a)** all available DB data at 1 May 2006, **(c)** all available DB data at 2 May 2006, **(e)** all available DB data at 3 May 2006. **(b)**, **(d)**, and **(f)** are similar as **(a)**, **(c)**, and **(e)** correspondingly, but for data with QA equals to “very good” only.

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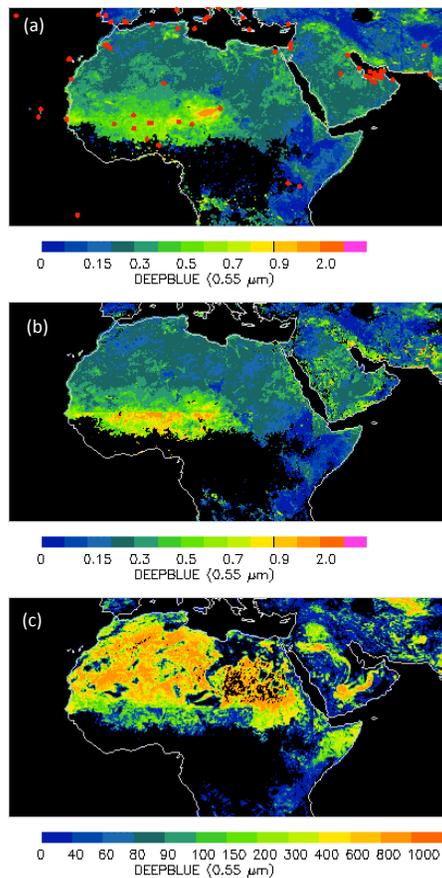


Fig. 6. Spatial distributions of DB for 2006 **(a)** AOD before the QA filtering, **(b)** AOD after the QA very good filtering, and **(c)** Number of pixel available after the QA filtering. Red dots in **(a)** represent the AERONET sites.

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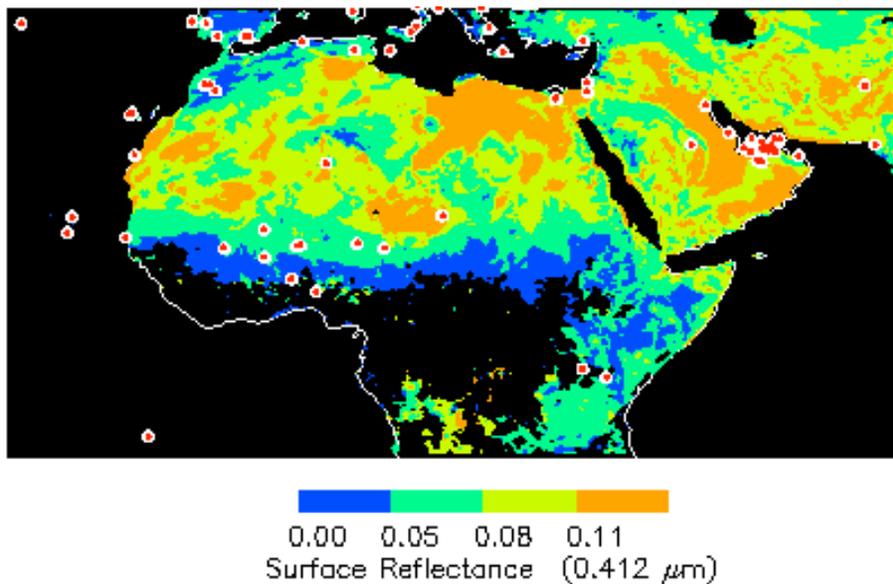


Fig. 9. Spatial distribution of the selected ranges of surface reflectance at $0.412 \mu\text{m}$. The four albedo ranges are 0–5 % (blue), 5–8 % (green), 8–11 % (yellow) and above 11 % (orange). The AERONET sites are represented by red dots that surrounded by white line.

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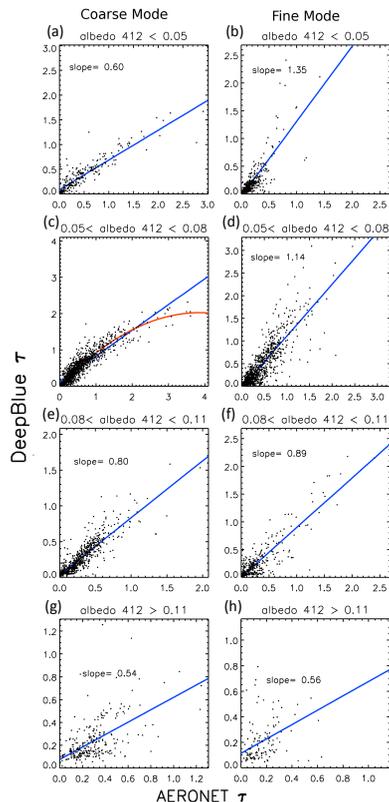


Fig. 10. Comparisons between coarse and fine mode Aqua DB AOD and AERONET AOD at $0.55 \mu\text{m}$ globally 2002–2009 with albedo at $0.412 \mu\text{m}$ **(a)** and **(b)** smaller than 0.5, **(c)** and **(d)** ranged between 0.5 and 0.8, **(e)** and **(f)** ranged between 0.8 and 0.11, and **(g)** and **(h)** greater than 0.11. The left panels show the coarse mode with fine mode fraction smaller than 0.5, the right panels show the fine mode fine mode fraction greater than 0.5. The blue line is the linear regression line and the red line is the polynomial regression line.

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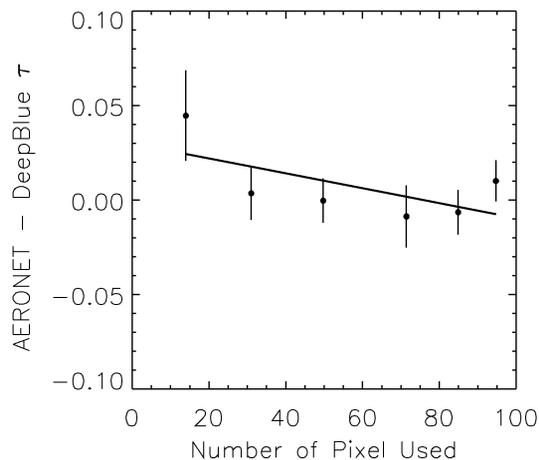


Fig. 11. AOD bias ($\Delta\tau_{A-M}$, AERONET minus DB AOD) as a function of number of pixel used in retrieving for Aqua DB over North Africa. The one standard deviation bar was shown.

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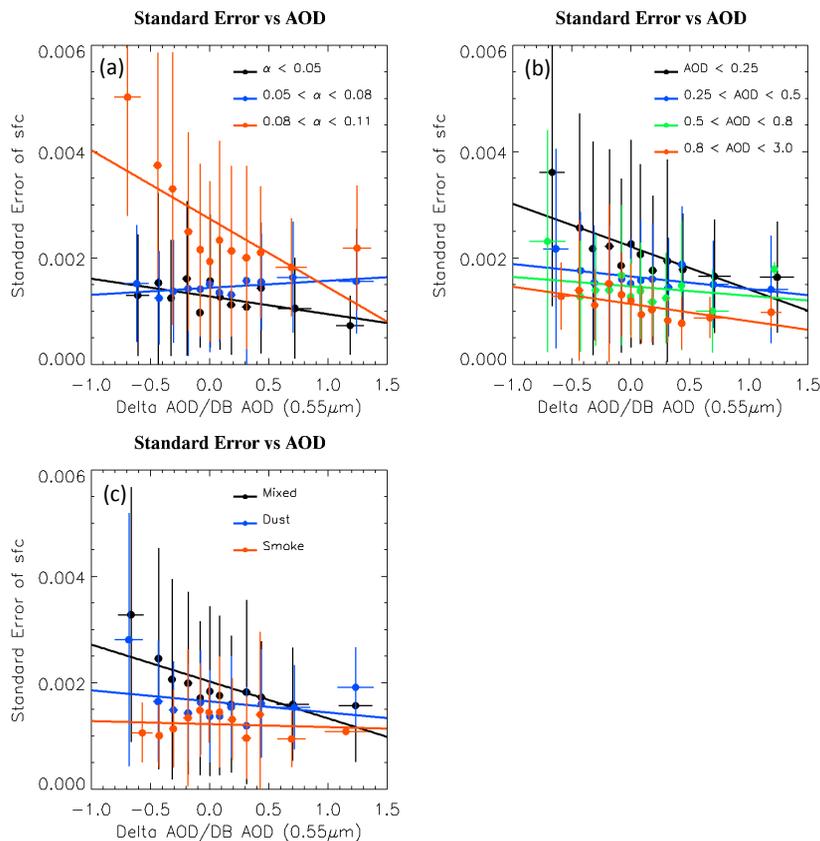


Fig. 12. Normalized ΔAOD ($\Delta\tau_{A-M}$ over DB AOD) various with STE_{sfc} as a function of **(a)** surface reflectance at 0.412 μ m, **(b)** DB AOD, and **(c)** aerosol type. The one standard deviation bar was shown.

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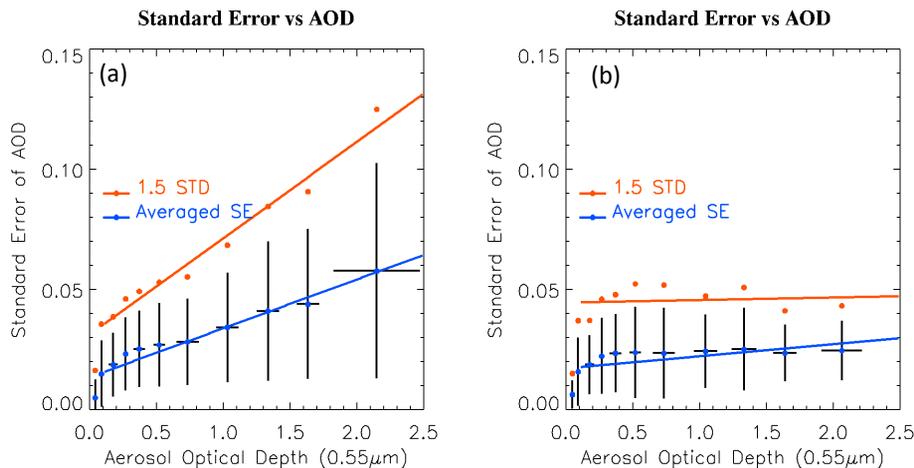


Fig. 13. Scatter plot of standard error threshold of Aqua AOD versus Aqua AOD at 0.55 μ m. Dots represent the averaged Standard Error (blue) of AOD and the 1.5 standard deviation (red) for every 0.05 of AOD when AOD < 0.5 and 0.3 of AOD when AOD > 0.5. The blue lines and red lines show the linear fit of corresponding dots. **(a)** for DB AOD globally. **(b)** for DB AOD over North Africa.

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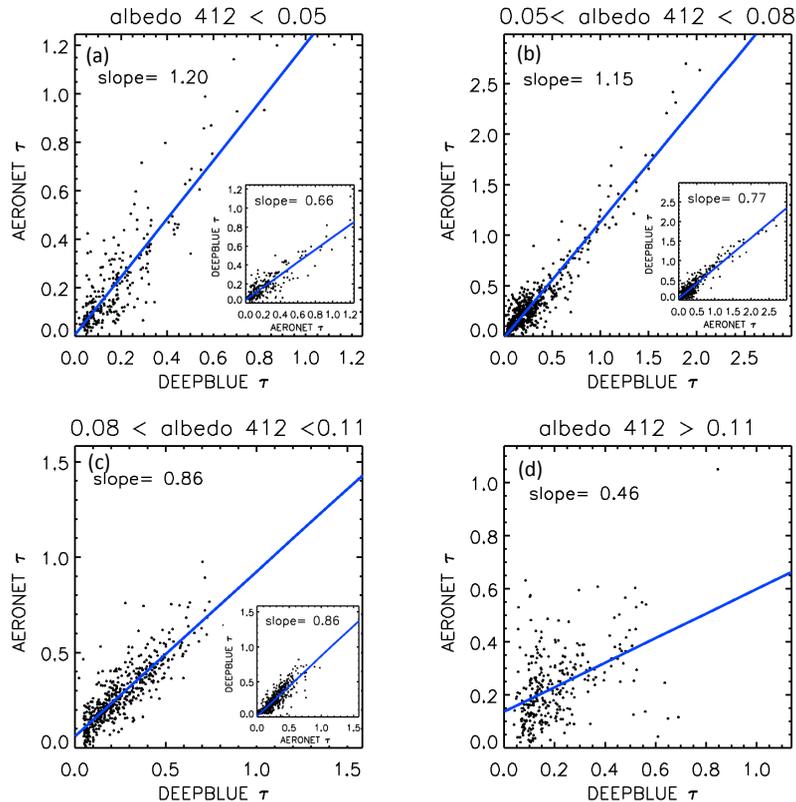


Fig. 14. Comparisons between Aqua DB and AERONET over North Africa 2002–2009 with albedo at $0.412\ \mu\text{m}$ for mixed aerosol type, **(a)** smaller than 0.5, **(b)** ranged between 0.5 and 0.8, **(c)** ranged between 0.8 and 0.11, and **(d)** greater than 0.11. The blue line is the polynomial or linear fit line.

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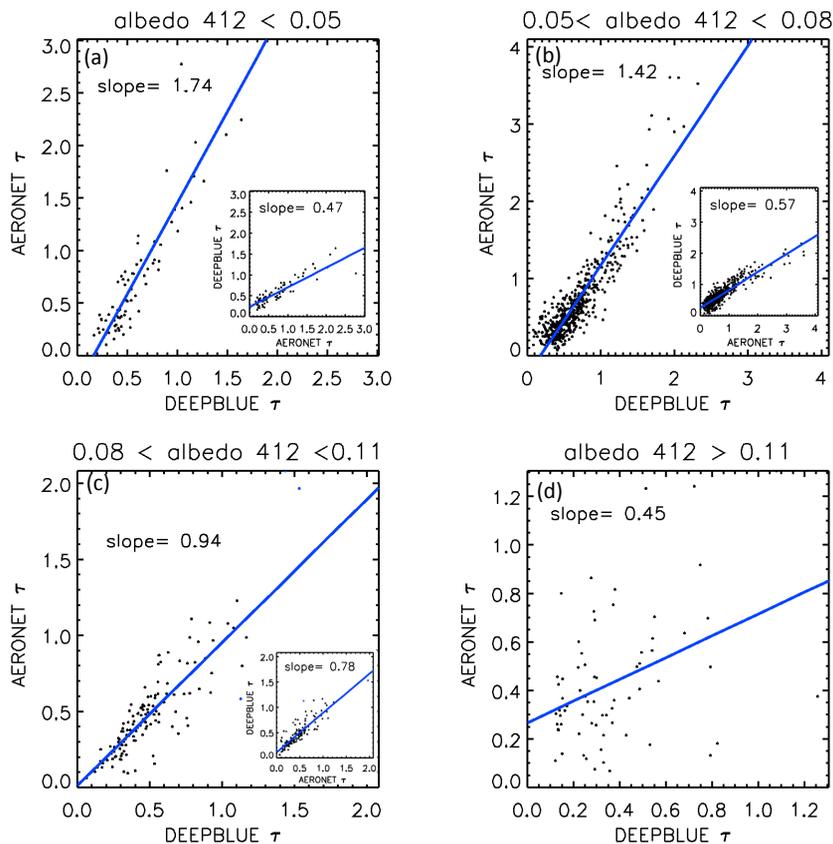


Fig. 15. Similar to Fig. 14 but for dust type aerosol over North Africa only.

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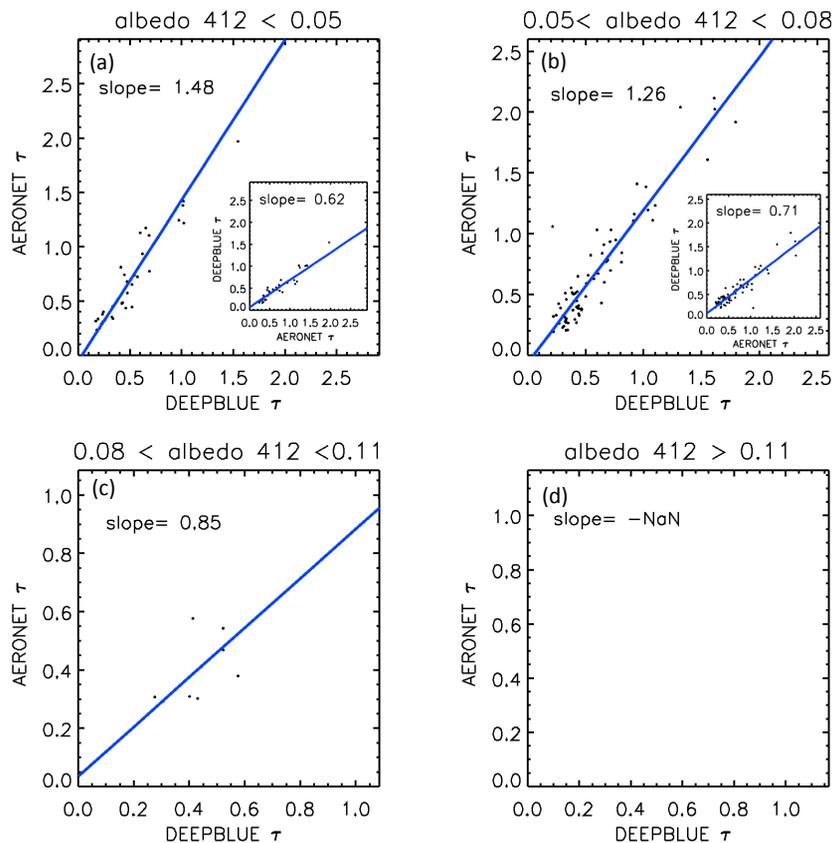


Fig. 16. Similar to Fig. 14 but for smoke type aerosol over North Africa only.

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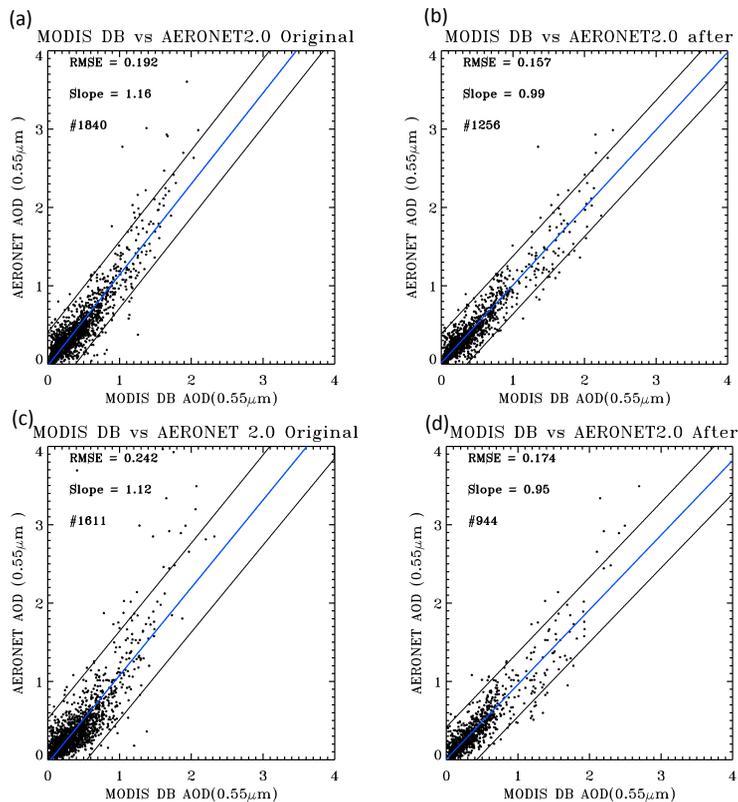


Fig. 17. Scatter plot of DB AOD versus AERONET level 2.0 AOD at 0.55 μm. The blue line is the linear regression line for all data and the black lines are the 1.0 standard deviation line of the blue line. **(a)** for the original Aqua DB aerosol products, **(b)** for the DA-quality Aqua DB aerosol products, **(c)** and **(d)** are similar to **(a)** and **(b)** but for Terra DB.

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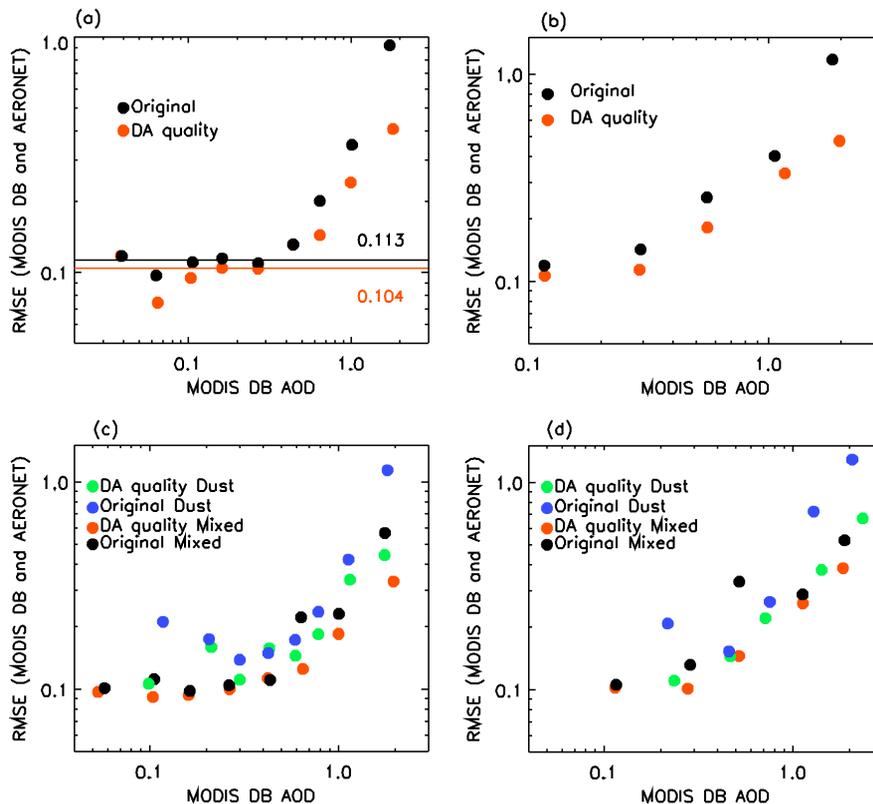


Fig. 18. RMSE of DB AOD comparing to AERONET AOD as a function of DB AOD for all data and for mixed and dust aerosol types for Aqua (a and c) and for Terra (b and d). The RMSE of original and DA-quality mixed and dust aerosols are indicated with the different color dots.

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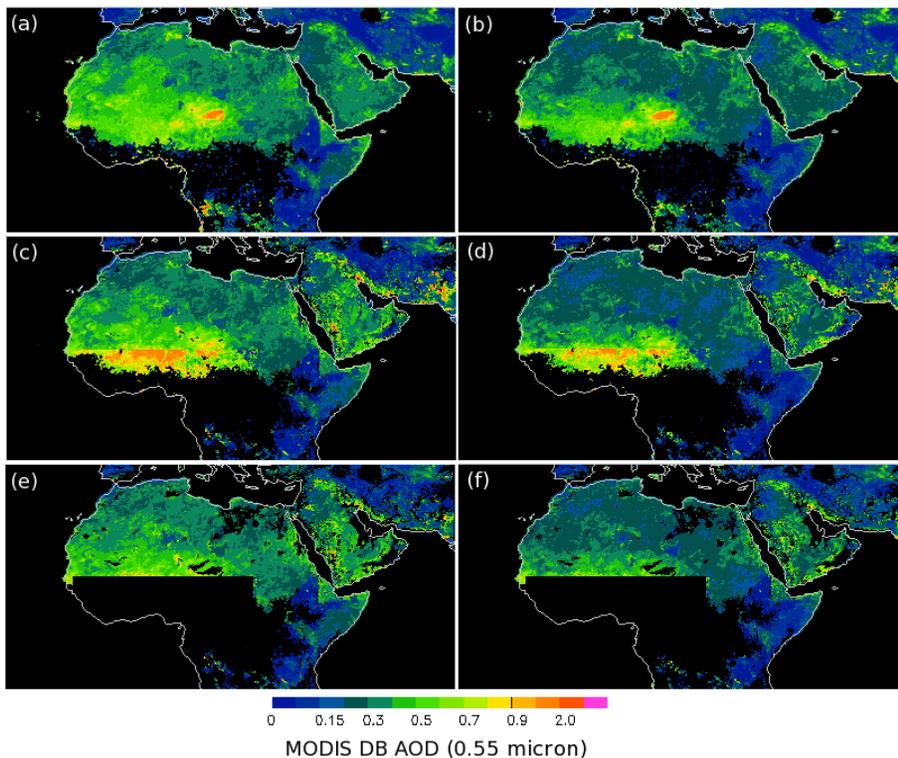


Fig. 19. Spatial distribution of AOD at 0.55 μm from the DB aerosol products for 2007. The black color represents regions with no data, the blue color represents areas with low AOD loadings, and the pink color indicates locations with extreme high AOD values. **(a)** for the original Terra DB data, **(c)** as in **(a)** but for Terra AOD with “very good” QA flags, and **(e)** as in **(a)** but for DA-quality Terra AOD. **(b)**, **(d)** and **(f)** as in **(a)**, **(b)**, and **(e)** but for Aqua.

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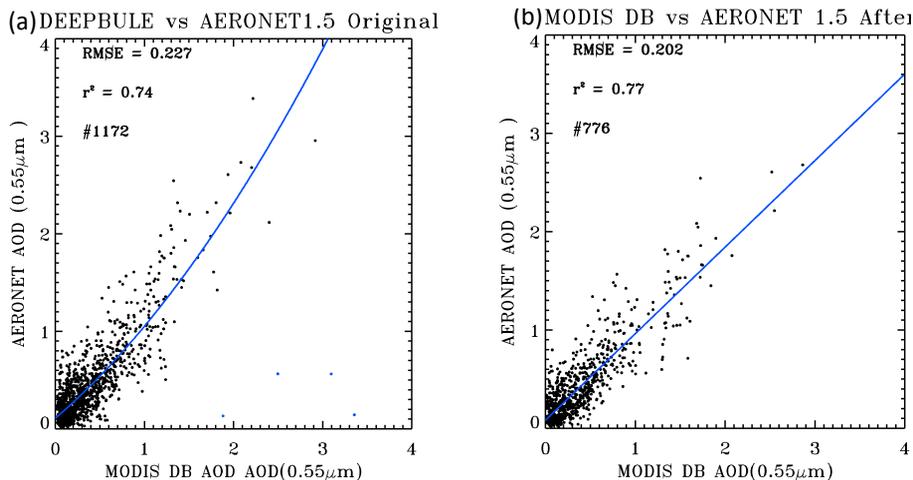


Fig. 20. Scatter plot of Aqua DB versus AERONET level 2.0 AOD at $0.55 \mu\text{m}$ over 2010 to 2011 for independent study. The blue line is the polynomial/linear regression line for all data and the black lines are the 1.0 standard deviation line of the blue line. **(a)** For the original Aqua DB aerosol products, **(b)** for the DA-quality Aqua DB aerosol products.

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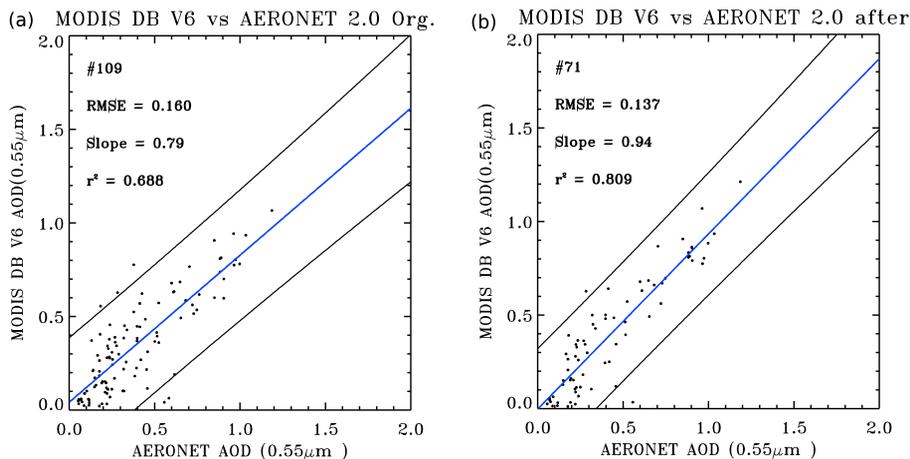


Fig. 21. Scatter plot of MODIS Aqua DB preliminary c6 versus AERONET level 2.0 AOD at $0.55\ \mu\text{m}$ for April 2006 and July 2008. The blue line is the linear regression line for all data and the black lines are the 1.0 standard deviation line of the blue line. **(a)** For the preliminary DB v6 aerosol products, **(b)** for the modified Aqua DB aerosol products using procedures that developed based on DB c5.1 data.

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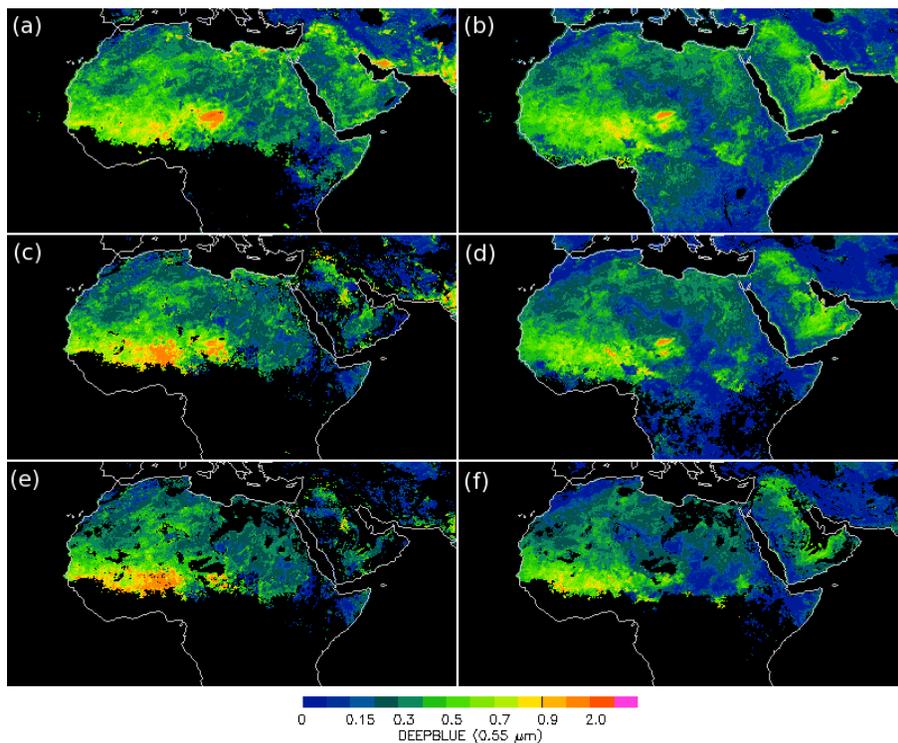


Fig. 22. Spatial distribution of AOD at $0.55\ \mu\text{m}$ from the DB aerosol products for April 2006. The black color represents regions with no data, the blue color represents areas with low AOD loadings, and the pink color indicates locations with extreme high AOD values. **(a)** For the original Aqua DB c5.1 data, **(c)** as in **(a)** but for Aqua c5.1 AOD with “very good” QA flags, and **(e)** as in **(a)** but for DA-quality Aqua c5.1 AOD. **(b)**, **(d)** and **(f)** as in **(a)**, **(b)**, and **(e)** but for Aqua DB preliminary c6 data.