Improvement of aerosol optical depth retrieval from MODIS spectral reflectance over the global ocean using new aerosol models archived from AERONET inversion data and tri-axial ellipsoidal dust database

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Abstract. New over-ocean aerosol models are developed by integrating the inversion data from the Aerosol Robotic Network (AERONET) sun/sky radiometers with a database for the optical properties of tri-axial ellipsoid particles. The new aerosol models allow more accurate retrieval of aerosol optical depth (AOD) from the Moderate Resolution Imaging Spectroradiometer (MODIS) in the case of high AOD (AOD > 0.3). The aerosol models are categorized by using the fine-mode fraction (FMF) at 550 nm and the single-scattering albedo (SSA) at 440 nm from the AERONET inversion data to include a variety of aerosol types found around the globe. For each aerosol model, the changes in the aerosol optical properties (AOPs) as functions of AOD are considered to better represent aerosol characteristics. Comparisons of AODs between AERONET and MODIS for the period from 2003 to 2010 show that the use of the new aerosol models enhances the AOD accuracy with a Pearson coefficient of 0.93 and a regression slope of 0.99 compared to 0.92 and 0.85 calculated using the MODIS Collection 5 data. Moreover, the percentage of data within an expected error of ±(0.03 + 0.05 × AOD) is increased from 62% to 64% for overall data and from 39% to 51% for AOD > 0.3. Errors in the retrieved AOD are further characterized with respect to the Ångström exponent (AE), scattering angle (Θ), SSA, and air mass factor (AMF). Due to more realistic AOPs assumptions, the new algorithm generally reduces systematic errors in the retrieved AODs compared with the current operational algorithm. In particular, the underestimation of fine-dominated AOD and the scattering angle dependence of dust-dominated AOD are significantly mitigated as results of the new algorithm’s improved treatment of aerosol size distribution and dust particle nonsphericity.

1 Introduction

Aerosols exert a significant impact on climate change and air quality. The small airborne particles regulate the radiation budget through both direct and indirect effects (IPCC, 2007), specifically, by scattering and absorbing radiation and by modifying cloud microphysics. Aerosols are known to affect human health by causing and worsening respiratory illnesses (Pope and Dockery, 2006). Because the spatio-temporal distribution of aerosols is highly variable, satellite observations have been extensively utilized to quantify aerosol optical properties (AOPs) over wide areas and with fine spatio-temporal resolution.
Traditional 5-channel meteorological imagers, including single visible-band instruments aboard geostationary satellites, are used to continuously monitor aerosol optical depth (AOD), but have a limited ability to retrieve other parameters (Knapp et al., 2002; Wang et al., 2003; Kim et al., 2008). In contrast, multi-spectral instruments on board low Earth orbit (LEO) satellites, such as the Advanced Very High Resolution Radiometer (AVHRR), Sea-viewing Wide Field-of-view Sensor (SeaWiFS), and Moderate Resolution Imaging Spectroradiometer (MODIS), can retrieve aerosol size information and absorptivity (Higurashi and Nakajima, 1999, 2002; Mishchenko et al., 1999; Hsu et al., 2004, 2006; Remer et al., 2005; Kim et al., 2007; Levy et al., 2007b). The Geostationary Ocean Color Imager (GOCI), which observes spectral radiances centered at 412, 443, 490, 555, 660, 680, 745, and 865 nm from a geostationary orbit, has been used for hourly monitoring of AOD and to retrieve the fine-mode fraction (FMF) and aerosol types over East Asia (Lee et al., 2010b).

With their wide spatial and spectral coverage, the observations made by the MODIS instruments aboard the Terra and Aqua satellites provide an unprecedented opportunity to infer AOPs. MODIS has 36 spectral bands ranging from 0.41 to 15 µm with three different spatial resolutions (250 m, 500 m, 1 km) and with 2300 km-wide swath coverage. Since the launch of MODIS in 1999 for Terra and 2002 for Aqua, numerous efforts have been made to retrieve, evaluate, and improve the aerosol products obtained. The original operational algorithms for dark vegetated areas (Kaufman et al., 1997) and oceans (Tanré et al., 1997) are two very important additions. The MODIS algorithms have been frequently updated to improve the quality of retrieved data by modifying cloud-masking processes, aerosol models, and the surface reflectance databases (Remer et al., 2005; Levy et al., 2007a, b). Hsu et al. (2006) developed Deep-Blue algorithm, which is applicable to bright land surfaces including desert areas, to facilitate monitoring of dust aerosols over source regions. Consequently, the current MODIS operational algorithms provide the columnar aerosol amount (AOD) and size information (FMF, Ångström exponent [AE]) for full coverage of the Earth except for cloud- and snow-covered areas. In addition, the Deep-Blue algorithm also has the ability to retrieve the single-scattering albedo (SSA) of dust aerosols.

MODIS aerosol products have been validated extensively to evaluate data quality. Preliminary comparisons of AOD from Terra-MODIS with that observed from Aerosol Robotic Network (AERONET) Sun/sky radiometers (Holben et al., 1998) showed that the AOD at 660 nm over the ocean differed by only 2% on average, with negligible offset (Remer et al., 2002), while the Terra-MODIS AOD over land was underestimated by about 14% except for coastal areas (Chu et al., 2002). However, the comparison results for land varied significantly with location, partially due to different surface conditions and aerosol sources. On the contrary, a validation by Remer et al. (2008) showed an almost perfect regression slope for the AOD at 550 nm over land as calculated by AERONET and MODIS, but an underestimation of AOD over the ocean from Aqua-MODIS, in particular for high AODs. It should be noted that the land algorithm has been modified substantially to resolve better aerosol models and surface reflectance (Levy et al., 2007a, b), whereas no substantial update has been made to the original ocean algorithm (Remer et al., 2005, 2006). Therefore, the significant improvement in the regression slope over land is likely attributed to improved aerosol models to some extent, because the slope largely depends on data in the high AOD regime where the aerosol signal dominates the surface signal.

In this paper, new aerosol models are introduced by integrating AERONET inversion data (Dubovik and King, 2000; Dubovik et al., 2006) with single-scattering property data from a tri-axial ellipsoid database (Meng et al., 2010). The AOPs of each aerosol model are used to calculate a lookup table (LUT) for spectral reflectances from MODIS. By using the LUT, retrieval and validation of AODs are performed over the global ocean using Aqua-MODIS data to improve the underestimation of AOD reported by Remer et al. (2008). The validation results are compared with those from the current operational algorithm to further characterize the effects of the new aerosol models.

2 MODIS ocean algorithms

Remer et al. (2005, 2006) described the current MODIS Collection 5 operational over-ocean algorithm (hereafter, C005 algorithm) in detail. The algorithm retrieves spectral AOD and FMF using spectral reflectances centered at 555, 650, 860, 1240, 1630, and 2120 nm by comparing observed and pre-calculated reflectances. To this end, sophisticated forward radiative transfer simulations of the reflectances (i.e. LUT) need to be performed for various aerosol models, surface reflectances, and sun/satellite geometries. Because the top-of-atmosphere (TOA) reflectance consists of signals from both the surface and atmosphere, the algorithm specifies surface reflectance in terms of the Fresnel reflection accounting for sea-surface roughness with a wind speed of 6 m s⁻¹ and zero water-leaving radiance except at 550 nm where a water-leaving radiance of 0.005 is assumed. The atmospheric contribution, aerosols in particular, is calculated using four fine-mode and five coarse-mode aerosols. Then, both spectral AOD and FMF (550 nm), a ratio of fine-mode AOD to total AOD, are simultaneously retrieved by minimizing the error between the observed and calculated reflectances for each of the 20 combinations from the fine- and coarse-mode aerosol models with the fixed AOD retrieved from 860 nm.

A schematic flowchart of the C005 algorithm and a test algorithm to evaluate the effects of the new aerosol models introduced in this paper is provided in Fig. 1. The test algorithm is designed to use the same spectral reflectances as the C005 algorithm in order to constrain other effects that
can arise from different pre-processing of the data. We used the “Mean Reflectance_Ocean” product in the “MYD04” files, which provides cloud- and sediment-masked mean reflectance in 20 × 20 pixels of 500 m pixel-resolution data at seven wavelengths centered at 470, 555, 650, 860, 1240, 1630, and 2120 nm. The product is the same as that used in the C005 algorithm. The major difference between the two algorithms is the aerosol models used to calculate the LUT.

3 New aerosol models

Use of a radiative transfer model (RTM) to simulate satellite-observed TOA reflectance requires aerosol characteristics such as spectral refractive indices, size distribution, and nonsphericity to describe nonspherical particles. Otherwise, the spectral AOD, SSA, and phase function, which are derived from the aforementioned aerosol properties, are required. Thus, long-term AERONET inversion data that provides the AOPs for the globe can be used to simulate the satellite signal for various aerosol types. It should be noted that the AERONET observes ambient-columnar properties similar to those obtained from satellite observations, while in-situ measurements provide near-ground properties. Moreover, the AERONET-retrieved AOPs represent the radiation field well for a wide scattering angle range, because the inversion data are retrieved to match the calculated radiation field with the observed sky radiances from the combined principal/almucantar planes (Dubovik and King, 2000; Dubovik et al., 2006). The inversion data provide AOPs at 440, 675, 870, and 1020 nm, but for MODIS observations, the tri-axial ellipsoidal database, introduced in the work of Meng et al. (2010), is required to expand the wavelength range up to 2120 nm.

3.1 AERONET inversion data

The quality-assured, “Level 2 Inversion All Points” data are used to derive aerosol models over the ocean for the test algorithm. To this end, data needs to be collected from specific AERONET stations chosen by distance from the ocean. The distance from the ocean is calculated by using geo-location information for each AERONET site and a high-resolution digital elevation model (DEM). The criterion for selecting the coastal stations was the distance within 7 km from the ocean. Figure 2 shows the 81 selected stations and the number of inversion data available to date. Although large portions of the data are from the US and Europe, where anthropogenic aerosols are dominant, the AERONET data in
particle-dominated aerosols mainly represent dust events. Note that sea salt, non-absorbing coarse-mode aerosols, generally occurs with low AOD values. For fine particle-dominated aerosols (FMF > 0.6), the range of values for SSA is wider than that for coarse particle-dominated aerosols. The high SSA values correspond to non-absorbing anthropogenic aerosols, such as sulfates and nitrates; whereas, the low SSA values imply the presence of black carbon (BC) (Hess et al., 1998; Wang and Martin, 2007). The major difference between global and coastal data is highlighted by the lack of data in the extremely low SSA regime. The high relative humidity (RH) in coastal areas, the aging of BC during transport, and the few AERONET stations in downwind of biomass-burning aerosols may cause the result. Both high RH and BC aging are known to increase SSA (Wang and Martin, 2007).

Based on the representation of aerosol types classified using FMF and SSA (Lee et al., 2010a), aerosol models are created by quantized square-bins over the FMF and SSA domains. Binning intervals of 0.1 and 0.05 are used for FMF and SSA, respectively. Each aerosol model is further categorized as a function of AOD by averaging AOPs between fore- and aft-medians of each AOD nodal point. If no data exist for a higher AOD bin, the AOPs of the previous bin is used. Consequently, the spectral AOD, SSA, and phase function are averaged over the three-dimensional domains of FMF, SSA, and AOD to be used as input data for the LUT calculations. Prior to the averaging, spectral AOD is normalized by itself at 550 nm and multiplied by each AOD nodal point. This method, however, has limited application to low AOD data, because SSA is retrieved only for AOD (440 nm) > 0.4. As an alternative, the SSA is assumed to be 0.99, regardless of the wavelength, by considering the sea salt dominance in the low AOD regime over the ocean, while the other parameters (spectral AOD, phase function) are compiled from AERONET inversion data. For marine aerosol models used for AOD ≤ 0.15, only FMF criteria and AOD < 0.15 are used to calculate the AOPs, and SSA is assumed to be 0.99. As a result, a total of 23 aerosol models for AOD > 0.15 and 9 marine aerosol models for AOD ≤ 0.15 are created with the number of data points constrained to be greater than 10 for each aerosol model. The aerosol models cover FMF ranging from 0.2 to 1.0 for AOD ≤ 0.95 (16 types), from 0.3 to 1.0 for SSA > 0.95 (7 types), and from 0.1 to 1.0 (9 types) for marine aerosol models. Dimensions of the LUT are summarized in Table 1. Note that simple extrapolation is used to retrieve AOD of severe dust storms or smoke events with AOD higher than 3.6 (LUT limit).

3.2 Tri-axial ellipsoid database

The AERONET inversion data provide AOPs for wavelengths ranging from 440 to 1020 nm, while the MODIS observations cover the wavelengths from 470 to 2120 nm. To expand the wavelength range of AERONET AOPs, data
Fig. 3. The number of data points included in each FMF (550 nm) and SSA (440 nm) bin, archived from the AERONET inversion data over the globe (left) and coastal areas (right). The data were sorted into intervals of 0.05 and 0.01 for FMF and SSA, respectively. The AERONET stations in the coastal area are shown in Fig. 2.

Table 1. LUT dimensions for the MODIS over-ocean algorithm.

<table>
<thead>
<tr>
<th>Variable Name</th>
<th>No. of Entries</th>
<th>Entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wavelength ($\lambda$)</td>
<td>7</td>
<td>470, 555, 650, 860, 1240, 1630, 2120 nm (band 3, 4, 1, 2, 5, 6, 7, respectively)</td>
</tr>
<tr>
<td>SZA ($\theta_o$)</td>
<td>8</td>
<td>0, 10, …, 70°</td>
</tr>
<tr>
<td>SAZA ($\theta_s$)</td>
<td>8</td>
<td>0, 10, …, 70°</td>
</tr>
<tr>
<td>RAA ($\phi$)</td>
<td>19</td>
<td>0, 10, …, 180°</td>
</tr>
<tr>
<td>AOD ($\tau$)</td>
<td>9</td>
<td>0.0, 0.1, 0.3, 0.6, 1.0, 1.5, 2.1, 2.8, 3.6</td>
</tr>
<tr>
<td>Aerosol Model</td>
<td>23</td>
<td>Classified by FMF and SSA from AERONET inversion data</td>
</tr>
</tbody>
</table>

SZA: solar zenith angle, SAZA: satellite zenith angle, RAA: relative azimuth angle.

Table 1: LUT dimensions for the MODIS over-ocean algorithm.

The procedure to calculate the AOPs of the predefined aerosol models at the longer wavelengths ($\lambda \geq 1240$ nm) is summarized as follows:

1. Extracting extinction efficiency, SSA, and phase function for individual spherical/nonspherical particles from the database by inputting refractive indices, size parameter, and aspect ratios. Note that the RTM we used requires spectral AOD, SSA, and phase function to calculate TOA reflectances. The refractive indices for each aerosol model are from the MODIS operational algorithm since AERONET inversion data does not provide the values at the longer wavelengths.

2. Integrating the AOPs of individual particles using predefined size distributions by assuming spherical particles. The size distribution of each aerosol model is calculated by averaging AERONET inversion data the same as AOPs for the shorter wavelengths.

3. Doing the same procedure as (2) for pure nonspherical particles. Thus, integrating the AOPs of individual particles in both size distribution and aspect ratio distribution space. The same aspect ratio distribution as AERONET inversion algorithm is used for consistency with the AOPs calculated for the shorter wavelengths.

4. Calculating weighting mean of the AOPs for pure spheres and pure nonspherical particles using %sphericity. The mean values of %sphericity of each aerosol model are calculated by averaging AERONET inversion data.

from the tri-axial ellipsoid database (Meng et al., 2010) are used in this study. The database containing the single-scattering properties of individual tri-axial ellipsoidal particles was computed using the Lorentz-Mie code (Bohren and Huffman, 1983), the T-matrix code (Mishchenko and Travis, 1998), the Amsterdam discrete dipole approximation (DDA) code (Yurkin and Hoekstra, 2009), and the improved geometric optics method (IGOM) code (Yang and Liou, 1996; Yang et al., 2007; Bi et al., 2009). Because tri-axial ellipsoidal shapes include spheres and ellipsoids with a number of aspect ratios, the application of the database can be expanded to non-dust aerosols. The database provides extinction efficiency, SSA, phase matrix, etc., for various refractive indices, size parameters, and aspect ratios, thus the proxy of the AERONET AOPs (spectral AOD, SSA, and phase function) can be extracted when given the spectral refractive indices, size distribution, aspect ratios, and nonsphericity.

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More specifically, the refractive indices of “water soluble” and “water soluble with humidity” from the C005 aerosol models (Remer et al., 2006) are used for fine-mode (0.85 < SSA < 0.95 and SSA > 0.95, respectively), and the refractive indices of “dust-like type” and “wet sea salt type” are used for coarse-mode (AOD > 0.1 and AOD = 0.1, respectively). Although the refractive indices of the MODIS aerosol models are not completely consistent with those of the new aerosol models, the low sensitivity of satellite signals to the fine-mode aerosols at longer wavelengths (≥ 1240 nm) due to their low AOD (high AE) and the relatively well-known absorption properties of dust (almost non-absorbing) (Hsu et al., 2004; Remer et al., 2005) are expected to result in smaller errors compared to excluding the longer wavelengths in the retrieval algorithm. A test retrieval using only shorter wavelengths (not shown for brevity) showed that exclusion of the longer wavelengths resulted in larger uncertainties than its counterpart particularly for determining aerosol size information. Nonetheless, more accurate optical property information for the longer wavelengths is still desirable for further improvement in the aerosol models and thus retrieval results.

With regard to nonsphericity and aspect ratios, mean “% sphericity” from the AERONET data and fixed spheroid mixture distribution are used as described in Dubovik et al. (2006). The dataset compiled by combining the AERONET inversion data and tri-axial ellipsoid database data is used as input data into RTM calculations. The optical properties of the 23 aerosol models are summarized in Table 2. To calculate the LUT, a discrete ordinate radiative transfer (DISORT) code implemented into the libRadtran software package (Mayer and Kylling, 2005) is used. Due to the advantage of directly inputting the phase function into the libRadtran package, nonsphericity, which mainly affects phase function, can be readily handled with the software. However, the polarization effect is not included the same as in the C005 algorithm.

4 Sensitivity study

The possible differences in retrieved AOD between the C005 algorithm and test algorithm are analysed before applying the developed algorithm to actual TOA reflectance data. Figure 4 shows the difference in the calculated TOA reflectance values between the C005 aerosol models and the new aerosol models for different AOD values at 860 nm, the reference wavelength used in selecting aerosol models from the C005 algorithm. The other wavelengths show similar tendencies. The corresponding C005 aerosol models to the new aerosol models are created by combining the F2 (“water soluble”) and C8 (“Dust-like type”) aerosol models from Remer et al. (2006) for SSA < 0.95 and F4 (“Water soluble with humidity”) and C8 for SSA > 0.95 using FMF values from new aerosol models. Negative values are shown in line-fill.
to be selected by the retrieval procedure. The test is carried with one-standard deviation intervals. The comparison results in various geometries and the other variables, except the target variable, are averaged at each nodal point and shown as a proxy of observation data for the whole LUT dimensions shown in Table 1 (total 283 176 data points). Two different proxy data are created by adding maximum random error of 3% and 10%. Figure 5 compares the exact solutions and the retrieved results. The data points with regard to various geometries and the other variables, except the target variable, are averaged at each nodal point and shown with one-standard deviation intervals. The comparison results show that each aerosol model (i.e., FMF and SSA) can be retrieved with small errors for the 3% error case, while

the fine-mode of the new aerosol model counterparts for low AOD. As a result, general underestimation of AOD is expected from the C005 algorithm compared with the test algorithm, and this may have caused the underestimation of high AOD in the validation results represented in Remer et al. (2008).

A redundancy test is performed to ensure whether all the aerosol models result in distinct spectral reflectance feature to be selected by the retrieval procedure. The test is carried out by retrieving AOPs, using calculated TOA reflectances as a proxy of observation data for the whole LUT dimensions shown in Table 1 (total 283 176 data points). Two different proxy data are created by adding maximum random error of 3% and 10%. Figure 5 compares the exact solutions and the retrieved results. The data points with regard to various geometries and the other variables, except the target variable, are averaged at each nodal point and shown with one-standard deviation intervals. The comparison results show that each aerosol model (i.e., FMF and SSA) can be retrieved with small errors for the 3% error case, while
significant misselection occurs for the 10% error case. The wrong retrieval is more prominent for SSA than FMF, showing lower accuracy in retrieving absorptivity than size information from MODIS. However, all the aerosol models are still required for the retrieval since highly-absorbing and non-absorbing aerosols are still discernable in some degree even for 10% error case.

5 Results and evaluation

The effects of the new aerosol models on AOD retrieval are evaluated by comparing the AODs from AERONET and MODIS data retrieved by the C005 and the test algorithm. Eight years of spectral reflectance data (2003–2010) observed from Aqua-MODIS are collected and processed to retrieve AOD using the new aerosol models. The AOD data from the C005 algorithm are also processed to compare with the AERONET observations, thereby allowing validation results from both algorithms to be compared. In this study, the “Effective_Optical_Depth_Average_Ocean” data in the MYD04 files are used for the C005 algorithm. Overall statistical scores and systematic errors are compared to characterize various error sources.

5.1 Overall evaluation

Figure 6 compares AODs between AERONET and MODIS over the global ocean from 2003 to 2010. Three different results retrieved from the C005 algorithm and the test algorithm using two different inversion procedures described in Sect. 2 are shown to investigate effects of new aerosol models and inversion methods on AOD retrieval accuracy. For this comparison, collocation was made within ±30 min in time and 25 km in space similar to the method proposed by Ichoku et al. (2002). However, we sampled satellite pixels by calculating actual distances between each AERONET location and the MODIS pixels for both test and operational datasets, while Ichoku et al. (2002) selected 5 × 5 MODIS pixels with an AERONET station located in the middle of the grid regardless of viewing angle. A criterion is applied for the number of data points, which requires at least 5 and 2 data points for MODIS and AERONET, respectively. Because the test algorithm tended to retrieve more data than the
Fig. 6. Comparison of AOD between AERONET and MODIS over the global ocean for the period from 2003 to 2010. The MODIS AODs are from the C005 algorithm (left) and the test algorithm (middle and right) with new aerosol models. Two different inversion procedures using standard deviation of spectral AOD (middle) and MODIS operational inversion (right) are applied for the test algorithm. The collocation criteria of ±30 minutes in time and 25 km in space were used. The gray dots represent all data points, whereas black dots with one-standard deviation interval represent mean AODs in 20 equal-number-of-data bins with respect to the AERONET data. The solid line is from the regression equation, while the dotted and dashed lines are the one-to-one line and the MODIS expected error (EE) line showing ±(0.03 + 0.05 × AOD), respectively. Only data points overlapping between the two algorithms are compared. Originally, the number of data points was 3106 for the C005 algorithm and 3578 for the test algorithm. The statistics shown are the Pearson coefficient ($R$), root mean squared error (RMSE), mean bias (MB), and the number of data points ($N$).

Table 3. Statistics for a comparison of AOD retrieved from the MODIS C005 algorithm and AERONET observations from 2003 to 2010 over the global ocean. The numbers in the parentheses are for AOD (AERONET) > 0.3.

<table>
<thead>
<tr>
<th>MODIS OP</th>
<th>2003</th>
<th>2004</th>
<th>2005</th>
<th>2006</th>
<th>2007</th>
<th>2008</th>
<th>2009</th>
<th>2010</th>
<th>Overall</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R$</td>
<td>0.91</td>
<td>0.93</td>
<td>0.92</td>
<td>0.87</td>
<td>0.94</td>
<td>0.92</td>
<td>0.92</td>
<td>0.94</td>
<td>0.92</td>
</tr>
<tr>
<td>Slope</td>
<td>0.78</td>
<td>0.87</td>
<td>0.82</td>
<td>0.77</td>
<td>0.9</td>
<td>0.9</td>
<td>0.88</td>
<td>0.87</td>
<td>0.85</td>
</tr>
<tr>
<td>y-intercept</td>
<td>0.04</td>
<td>0.02</td>
<td>0.03</td>
<td>0.04</td>
<td>0.02</td>
<td>0.03</td>
<td>0.03</td>
<td>0.03</td>
<td>0.03</td>
</tr>
<tr>
<td>Percentage</td>
<td>66%</td>
<td>62%</td>
<td>62%</td>
<td>62%</td>
<td>58%</td>
<td>62%</td>
<td>64%</td>
<td>65%</td>
<td>62%</td>
</tr>
<tr>
<td>within EE</td>
<td>(38%)</td>
<td>(37%)</td>
<td>(40%)</td>
<td>(40%)</td>
<td>(28%)</td>
<td>(43%)</td>
<td>(44%)</td>
<td>(54%)</td>
<td>(39%)</td>
</tr>
<tr>
<td>RMSE</td>
<td>0.06</td>
<td>0.07</td>
<td>0.05</td>
<td>0.05</td>
<td>0.06</td>
<td>0.06</td>
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</tr>
<tr>
<td>MB</td>
<td>(0.11)</td>
<td>(0.13)</td>
<td>(0.09)</td>
<td>(0.10)</td>
<td>(0.11)</td>
<td>(0.10)</td>
<td>(0.07)</td>
<td>(0.07)</td>
<td>(0.11)</td>
</tr>
<tr>
<td>$N$</td>
<td>393</td>
<td>451</td>
<td>441</td>
<td>346</td>
<td>377</td>
<td>336</td>
<td>347</td>
<td>264</td>
<td>2955</td>
</tr>
</tbody>
</table>

C005 algorithm due to the absence of a quality-control procedure used in C005 algorithm, only overlapping data retrieved by both algorithms were used for quantitative comparisons.

The validation results show that the AOD data from the C005 algorithm are highly correlated with the observations, but, on average, tend to be underestimated, with a Pearson coefficient of 0.92 and a regression slope of 0.85. The negative bias of the slope is caused by overestimation in the low AOD regime (AOD < 0.2) and underestimation in the high AOD regime (AOD > 0.3). Meanwhile, the new aerosol models improve the slope significantly (0.99–1.02) with a comparable correlation coefficient (0.93) regardless of the inversion methods. Only small differences are observed between the two results, showing a slight increase in statistics for the new inversion compared with the C005 inversion. However, the new inversion may not guarantee improved results for the C005 algorithm because of differences in the LUT. Since the difference is negligible between the two methods, only results from the new inversion will be shown for further analyses. From the statistics summarized in Tables 3 and 4, the aerosol models clearly improve almost all the statistics analysed in this study. The slope and the percentage of data within an expected error improved from 62 % to 64 % overall and from 39 % to 51 % for AOD > 0.3. These improvements are particularly noticeable for the high AOD regime at which the aerosol signal dominates the other contributions, such as Rayleigh scattering and surface reflectance. The major reason for the improvement in AOD
Table 4. Same as in Table 3 except for the test algorithm.

<table>
<thead>
<tr>
<th></th>
<th>This study</th>
<th>2003</th>
<th>2004</th>
<th>2005</th>
<th>2006</th>
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<th>2008</th>
<th>2009</th>
<th>2010</th>
<th>Overall</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R$</td>
<td></td>
<td>0.94</td>
<td>0.96</td>
<td>0.93</td>
<td>0.88</td>
<td>0.94</td>
<td>0.92</td>
<td>0.93</td>
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<td>0.93</td>
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<tr>
<td>Slope</td>
<td></td>
<td>1.01</td>
<td>1.00</td>
<td>0.97</td>
<td>0.91</td>
<td>1.01</td>
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Fig. 7. AE dependence of retrieval errors for the C005 algorithm (left) and the test algorithm (right) for overall data (upper) and data for AOD > 0.3 (lower). The data are sorted in 20 and 10 equal-number-of-data bins for the overall case and high AOD case, respectively. The dots and bars represent mean and one-standard deviation intervals of the retrieval errors, respectively, while the triangles represent the mean AOD from AERONET in each bin.

retrieval is the consideration of absorbing fine-mode aerosols and changing the size distribution as a function of AOD. Both factors are expected to increase AOD for a given TOA reflectance as shown in Fig. 4 and other previous studies (Levy et al., 2007b; Wang and Martin, 2007; Jethva et al., 2010). Note that the current MODIS algorithm adopts four different water-soluble aerosol models with fixed radii insensitive to AOD for the fine-mode cluster.

5.2 Error characteristics

Errors in AOD can arise from various sources including incorrect assumptions about surface reflectance and aerosol type, status of sensor calibration, observation geometry, etc. In addition, specific observation environments can bias results. Levy et al. (2010) evaluated the C005 over-land AOD data with regard to AE, cloud fraction, surface type
characteristics, and observation geometry to characterize systematic error sources. Thus, the analyses to be presented here together with the work of Levy et al. (2010) represent a complete evaluation of the MODIS data retrieved over land and ocean.

Figure 7 shows the AE dependence of the retrieval errors for the C005 and the test algorithms. The data were sorted into 20 and 10 equal-number-of-data bins for the overall data and AOD > 0.3, respectively. As shown in the result, the C005 algorithm tends to overestimate coarse-dominated AOD (AE < 0.8) and underestimate fine-dominated AOD (AE > 1.6). The underestimation of fine-dominated AOD worsens for high AOD cases, suggesting that the underestimation of high AOD from the C005 algorithm shown in Fig. 6 is mainly caused by fine-dominated cases, while reliable retrievals are performed for dust aerosols. The retrieved AODs are less stable (stability inferred by the magnitude of one standard deviation interval) for fine-dominated AOD than coarse-dominated AOD, while stable retrieval is observed for 0.75 < AE < 1.4 partially due to the relatively low AOD. In the case of AOD > 0.3, although there are systematic underestimations, the algorithm shows small mean biases (MBs) for strong dust events (AE < 0.4) with a higher stability than the fine-dominated case (AE > 1.4).

The AE dependence of MB for the test algorithm is reduced overall compared with the C005 algorithm, but the test algorithm still has a tendency to overestimate coarse-dominated AOD and to underestimate fine-dominated AOD. The AE dependence is reduced further for AOD > 0.3, but the AODs are distinctly overestimated for a coarse-dominated case (AE < 0.3). The improvement in the fine-dominated AOD for a high AOD case can be explained by the inclusion of the absorbing aerosol models and size distribution shift. As shown in Fig. 4, both effects can result in overestimation of AOD. In this case, the overestimation resulted in an improvement in underestimated AOD from the C005 algorithm. However, the standard deviation of the retrieval errors is slightly lower than that of the C005 algorithm for the coarse-dominated regime, while the standard deviation is similar between the two algorithms for the fine-dominated regime (AE > 1.3). As a result, the new aerosol models can be inferred to mitigate systematic errors (i.e., MB) compared with the C005 algorithm except for severe dust events (AOD > 0.3, AE < 0.3).

Figure 8 shows the scattering angle dependence of the retrieval errors. For the overall case of the C005 algorithm, the MB decreases gradually with increasing scattering angle and mean AOD. The decrease is a result of
combined effects of the systematic overestimation of low AOD cases (AOD < 0.2) and the underestimation of fine-dominated AOD with increasing AOD. In contrast, the scattering angle dependence of the MB is much lower in the test algorithm, indicating improved retrieval accuracy. Only two distinct positive peaks are present for 140° < Θ < 165°. For AOD > 0.3, the C005 algorithm shows systematic underestimation, while the test algorithm shows positive MB for Θ > 140° and negative MB for Θ < 140°. The underestimation in the C005 algorithm tends to worsen with increasing scattering angle, partially due to increasing AOD, while high AOD seems to correspond to low MB in the test algorithm.

For a more detailed explanation on the scattering angle dependence of the retrieval errors, additional comparisons for aerosol type information are shown in Fig. 9. Note that neglecting the nonsphericity of dust particles results in underestimation of AOD in the back-scattering direction, and overestimation in the side-scattering direction due to the difference in scattering phase function between spherical and nonspherical particles. For a dust-dominated case (AE < 0.8), the data provided by the C005 algorithm shows an imprint of the difference in phase functions between spherical and nonspherical particles, while the new aerosol models significantly reduce the scattering angle dependence. The new aerosol models, however, systematically overestimate the AOD regardless of the scattering angle. Consequently, the small MB of the C005 algorithm for coarse-dominated AOD, represented in Fig. 7, can be explained by cancellation of the positive and negative errors, while the test algorithm systematically overestimates AOD. For anthropogenic aerosols (AE > 1.2), neither algorithm shows distinct features related to differences in the phase function, while the systematic underestimation of the C005 algorithm in the back-scattering direction is significantly reduced by the test algorithm.

The retrieval results are further categorized with respect to the SSA in order to understand the impact of aerosol absorption on retrieval accuracy. Figure 10 shows the MB of the retrieved AODs for SSA. The AE constraint is also applied to separate fine-dominated and coarse-dominated cases. The daily mean SSA values from AERONET are used in this investigation since insufficient data points are gathered if a time constraint is applied. Note that AERONET Level 2 SSA values are retrieved for coarse-dominated cases. The daily mean SSA values from AERONET are used in this investigation since insufficient data points are gathered if a time constraint is applied. For anthropogenic aerosols (AE > 1.2), the C005 algorithm shows an imprint of the difference in phase functions between spherical and nonspherical particles. For a dust-dominated case (AE < 0.8), the data provided by the C005 algorithm shows an imprint of the difference in phase functions between spherical and nonspherical particles, while the new aerosol models significantly reduce the scattering angle dependence. The new aerosol models, however, systematically overestimate the AOD regardless of the scattering angle. Consequently, the small MB of the C005 algorithm for coarse-dominated AOD, represented in Fig. 7, can be explained by cancellation of the positive and negative errors, while the test algorithm systematically overestimates AOD. For anthropogenic aerosols (AE > 1.2), neither algorithm shows distinct features related to differences in the phase function, while the systematic underestimation of the C005 algorithm in the back-scattering direction is significantly reduced by the test algorithm.

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distinct dependence on SSA is observed for either dataset, but systematic overestimation of dust AOD from the test algorithm is highlighted. However, smaller standard deviations from the test algorithm indicate systematic error, while C005 algorithm shows somewhat larger dispersions. On the other hand, relatively strong absorptivity dependence is observed in the C005 algorithm for fine-dominated case, showing increasing underestimation tendency with SSA. In fact, the result is confusing because no highly absorbing aerosol model is included in the C005 algorithm and underestimation of absorptivity normally results in underestimation of AOD. However, the complexity of error sources can produce the anomaly. As found in this study, both absorptivity and particle size assumed in the retrieval algorithm can cause errors in the retrieved AOD. In addition, errors in the retrieved FMF can result in additional error in the AOD. The results from the test algorithm show relatively accurate AOD retrieval with mitigated SSA dependence.

The sensitivity of TOA reflectance to AOD increases with air mass because of the increasing optical path. Thus, the air mass factor (AMF), defined by \( m_{\text{Sun}} \times m_{\text{satellite}} \) where \( m = \sec(\theta) \), can affect retrieval accuracy. Figure 11 shows the retrieval error dependence on the AMF. We expected the retrieval errors to decrease with the AMF because of increased sensitivity; however, the pattern is more complicated because the retrieval errors are functions of AOD, \( \Theta \), and aerosol type. For both algorithms, retrieval stability increases (decreasing standard deviation) with the AMF partially because of increasing sensitivity. However, the MB shows different behavior; it decreases in the negative regime and then increases in the positive regime with increasing AMF for AMF < 1.6, and then gradually decreases with increasing AMF. For the high AOD case, however, a high AMF does not guarantee retrieval stability; the standard deviation is uncorrelated with the AMF. For the test algorithm, the MB tends to decrease with increasing AMF except for the bifurcation observed for AMF < 1.5, while no dependency is observed for the C005 algorithm.

6 Conclusions

We quantitatively assessed the impact of the use of new aerosol models on AOD retrieval from spectral reflectance observed by Aqua-MODIS over the global ocean for the period from 2003 to 2010. AERONET inversion data and the optical property data of tri-axial ellipsoidal dust particles from an existing database were used to compile AOPs in order to calculate LUTs, which include various aerosol types from absorbing to non-absorbing (0.85 < SSA < 1.00).
and from fine- to coarse-dominated (0.2 or 0.3 < FMF < 1.0). Because the MODIS C005 algorithm considers only water-soluble aerosols with/without humidity for fine-mode and sea salt/dust for coarse-mode, a noticeable difference was observed in AOD retrieval using the new algorithm with the consideration of various absorptivities and the size distribution change as a function of AOD.

Validation of the algorithms by using eight years of data revealed the new aerosol models to improve the AOD, with a regression equation of $y = 0.99x + 0.007$ and a Pearson coefficient of 0.93 compared to $y = 0.85x + 0.028$ and 0.92 for the C005 algorithm. The percentage of AOD data falling within the expected error was 64% for the test algorithm and 62% for the current operational algorithm. In particular, improvements were noted in the high AOD regime (AOD > 0.3) where the aerosol signal dominates the surface signal with a 12% increase in the number of reliable data points within the expected error. The root mean squared error (RMSE) and MB were also improved by the use of the new aerosol models.

To further characterize the retrieval errors, the data were validated with respect to AE, scattering angle, SSA, and AMF. The new aerosol models mitigated the dependence of MB (systematic error) on the aforementioned parameters. However, the coarse particle-dominated AOD was still overestimated and the fine particle-dominated AOD was underestimated. While the systematic overestimation of the coarse particle-dominated AOD increased for the high AOD case, the results for the fine particle-dominated AOD cases were similar compared to the overall case. Retrieval stability, however, was higher for the coarse particle-dominated case than the fine particle-dominated case, partially due to the wider variability in the optical properties of the fine-mode aerosols. In addition, the constrained analyses revealed the test algorithm to significantly reduce the scattering angle dependence of the retrieval error for dust-dominated cases (AE < 0.8, AOD > 0.3), partially due to improved treatment of the non-sphericity of dust particles and mitigated SSA dependence for fine-dominated cases. The standard deviation of the retrieval errors for the overall case tended to decrease with AMF as expected, but no distinct tendency was observed for AOD > 0.3. Our validation results indicate that the aerosol models adopted in the current MODIS operational algorithm need to be updated to achieve better accuracy. Further analyses on FMF and SSA retrievals are required to obtain a better understanding of the various error sources contributing to AOD retrieval and corresponding improvements in the aerosol retrieval algorithms.

Fig. 11. Air-mass factor ($m_{\text{Sun}} \times m_{\text{satellite}}$, where $m = \sec(\theta)$) dependence of retrieval errors for the C005 algorithm (left) and the test algorithm (right) for overall data (upper) and data for AOD > 0.3 (lower).
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