

1 **Analysis of the MODIS Above-Cloud Aerosol Retrieval**

2 **Algorithm Using MCARS**

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## 13 **Abstract**

14       The Multi-sensor Cloud and Aerosol Retrieval Simulator (MCARS) presently produces  
15 synthetic radiance data from Goddard Earth Observing System version 5 (GEOS-5) model  
16 output as if the Moderate Resolution Imaging Spectroradiometer (MODIS) was viewing a  
17 combination of atmospheric column inclusive of clouds, aerosols and a variety of gases and  
18 land/ocean surface at a specific location. In this paper we use MCARS to study the MODIS  
19 Above-Cloud AEROSol retrieval algorithm (MOD06ACAERO). MOD06ACAERO is  
20 presently a regional research algorithm able to retrieve aerosol optical thickness over clouds,  
21 in particular absorbing biomass burning aerosols overlying marine boundary layer clouds in  
22 the Southeastern Atlantic Ocean. The algorithm's ability to provide aerosol information in  
23 cloudy conditions makes it a valuable source of information for modeling and climate studies  
24 in an area where current clear sky-only operational MODIS aerosol retrievals effectively have  
25 a data gap between the months of June and October. We use MCARS for a verification and  
26 closure study of the MOD06ACAERO algorithm. The purpose of this study is to develop a set  
27 of constraints a model developer might use during assimilation of MOD06ACAERO data.

28       Our simulations indicate that the MOD06ACAERO algorithm performs well for marine  
29 boundary layer clouds in the SE Atlantic provided some specific screening rules are observed.  
30 For the present study, a combination of five simulated MODIS data granules was used for a  
31 dataset of 13.5 million samples with known input conditions. When pixel retrieval uncertainty  
32 was less than 30%, optical thickness of the underlying cloud layer was greater than 4 and  
33 scattering angle range within the cloud bow was excluded, MOD06ACAERO retrievals  
34 agreed with the underlying ground truth (GEOS-5 cloud and aerosol profiles used to generate  
35 the synthetic radiances) with a slope of 0.913, offset of 0.06, and RMSE=0.107. When only  
36 near-nadir pixels were considered (view zenith angle within +/-20 degrees) the agreement  
37 with source data further improved (0.977, 0.051 and 0.096 respectively). Algorithm closure

38 was examined using a single case out of the five used for verification. For closure, the  
39 MOD06ACAERO code was modified to use GEOS-5 temperature and moisture profiles as  
40 ancillary. Agreement of MOD06ACAERO retrievals with source data for the closure study  
41 had a slope of 0.996 with offset -0.007 and RMSE of 0.097 at pixel uncertainty level of less  
42 than 40%, illustrating the benefits of high-quality ancillary atmospheric data for such  
43 retrievals.

## 44 **1 Introduction**

45  
46 The MODerate resolution Imaging Spectroradiometer (MODIS) (Barnes et al., 1998) has  
47 proven to be an important sensor for aerosol data assimilation purposes for models such as the  
48 Goddard Earth Observing System Model, Version 5 (GEOS-5; Rienecker et al. 2008, Molod  
49 et al. 2012). There are two MODIS instruments on board NASA's Earth Observing System  
50 (EOS) *Terra* and *Aqua* spacecraft. There is a wide variety of data products available from  
51 these instruments for Land, Ocean and Atmosphere disciplines. Atmosphere discipline  
52 products include cloud mask, cloud top properties, cloud optical and microphysical properties  
53 and atmospheric aerosol properties. The MODIS data product files use a designation of MOD  
54 for Terra MODIS and MYD for Aqua MODIS. In this paper for brevity we will use "MOD"  
55 to refer to both instruments.

56 The largest contributor of biomass burning aerosols is Southern Africa (Reid et al, 2009,  
57 van der Werf et al, 2010, Chang et al, 2021). Biomass burning occurring from June through  
58 October creates thick smoke plumes that extend over the adjacent Atlantic Ocean. Prevailing  
59 winds in the area transport the smoke over the Southeast Atlantic Ocean (SEAO) and then as  
60 far as the Americas (Swap et al., 1996). The same time period coincides with a near-persistent  
61 layer of marine boundary-layer (MBL) stratus cloud that extends for several hundred miles  
62 westward from the Namibian coast (Devasthale and Thomas, 2011). The MODIS Dark Target  
63 aerosol retrieval algorithm (MOD04) that is used for ocean retrievals operates in clear sky  
64 conditions only. MOD04\_DT retrievals are not provided for each individual MODIS pixel-  
65 level, but rather are performed over a 3x3 or 10x10 set of pixels. Moreover aerosol properties  
66 are not retrieved over sun glint regions (Kaufman et al, 1997, Levy et al, 2009, 2013). The  
67 SEAO region has both extensive seasonal cloud cover and a significant portion of MODIS

68 granules containing sun glint, leading to equally extensive loss of continuous observations  
69 from the area.

70 Figure 1 illustrates these conditions using Terra MODIS data from 2006 through 2013.  
71 Panel a) shows the percentage of ocean gridboxes in the SEAO area that had daily mean cloud  
72 fraction greater than 50% in the MODIS Daily Level-3 gridded product (Hubanks, et al. 2019)  
73 stored at 1x1 degree resolution. Here, the SEAO area is defined the same way as in Meyer et  
74 al (2015), specifically between -20 and +20 degrees longitude and +4 to -20 degrees  
75 longitude. As much as 60% of all ocean gridboxes have cloud fraction greater than 50% in  
76 June (day 152) and only increase to the end of September (day 304). A 1-degree resolution  
77 gridbox will contain some clear sky and thus at least some aerosol retrievals are possible. As  
78 shown in Figure 1 b), in June between 70-80% of all ocean gridboxes contain some aerosol  
79 retrievals, though by September that number drops to between 30-50% year over year.

80 Due to aforementioned limitations of the standard dark-target MODIS aerosol algorithm,  
81 a model that assimilates aerosol data from SEAO would have very few aerosol retrievals over  
82 the ocean available to it. Most of the transport mechanism in the model would be thus  
83 governed by the model physical processes (e.g., advection, sedimentation and wet removal  
84 and vertical transport) instead of being constrained by observations.

85 The MOD06ACAERO algorithm (Meyer et al. 2015) fills in the aerosol data gap in  
86 SEAO as it is able to perform retrievals of aerosol properties above MBL clouds. The  
87 algorithm has been evaluated against observations from the Cloud-Aerosol Lidar and Infrared  
88 Pathfinder Satellite Observation (CALIPSO) (Winker et al, 2009), but CALIPSO only  
89 provides data at nadir and with a very limited spatial coverage. Recent improvements in  
90 CALIPSO version 4 aerosol products (Kim et al, 2018) indicate that the comparisons shown  
91 of the MOD06ACAERO algorithm with CALIPSO in Meyer et al (2015) would improve

92 somewhat as significant work had been done to remedy the low bias that CALIPSO retrievals  
93 have. However, Kim et al (2018) state that the remaining SEA low bias in CALIPSO  
94 retrievals of AOD with respect to AERONET and MODIS makes CALIPSO retrievals  
95 somewhat problematic as means of aerosol algorithm evaluation for SEAO area. (e.g., Meyer  
96 et al, 2013, 2015, Jethva et al, 2014). Observations collected during the ObserVations of  
97 Aerosols above CLouds and their IntEractionS (ORACLES) (Redemann et al, 2021) are  
98 currently being used to evaluate the MOD06ACAERO algorithm. Additional descriptions of  
99 ORACLES aerosol data can be found in LeBlanc et al (2020) and Pistone et al (2019).

100 In this study we applied an Observing System Simulation Experiment (OSSE) framework  
101 to gain insight on the performance of the MOD06ACAERO algorithm. Rather than using the  
102 classic analysis/forecast error metric common in Numerical Weather Prediction OSSE studies  
103 (e.g., Hoffman and Atlas 2016) we adopt here a “Retrieval OSSE” perspective where the  
104 quality of the retrieval is used as the verification metric (Wind et al. 2013, 2016). A radiative  
105 transfer code is applied to the model quantities combined with sensor geometry to simulate  
106 how a model scene appears to a specific instrument. A retrieval algorithm designed for that  
107 instrument can be executed on the simulated measurements. Physical quantities retrieved by  
108 the algorithm can be compared to the known simulation input. The algorithm can be examined  
109 for closure over a large spatial domain and thus any areas or conditions that may be  
110 problematic for the algorithm could be examined, and the strengths and limitations of the  
111 algorithm can be extensively documented.

112 The Multi-sensor Cloud and Aerosol Retrieval Simulator (MCARS) is a tool that  
113 combines model output with a radiative transfer code in order to simulate radiances that may  
114 be measured by a remote sensing instrument if it were passing over the model fields (Wind et  
115 al, 2013, 2016). In this paper, MCARS continues to use the combination of the GEOS-5

116 model, correlated- $k$  models of atmospheric transmittance due to various gaseous absorbers for  
117 MODIS channels as per Kratz (1995), inline Rayleigh scattering and the Discrete Ordinate  
118 Radiative Transfer (DISORT) code (Stamnes et al. 1988) to simulate MODIS radiances. Two  
119 improvements have been made to the MCARS code since last publication. The computational  
120 resolution has been increased to 32 streams, up from 16. Additionally, for this study the  
121 higher resolution 7 km GEOS-5 Nature Run (G5NR) was used in place of the standard 25 km  
122 resolution GEOS-5 output (Gelaro et al. 2015, da Silva et al. 2015, Putman et al. 2015).  
123 G5NR is a 2-year global, non-hydrostatic mesoscale model dataset for the period 2005-2006  
124 produced with the GEOS-5 Atmospheric GCM. The model run is performed at a horizontal  
125 resolution of 7 km using a cubed-sphere horizontal grid with 72 vertical levels, extending up  
126 to 0.01 hPa ( $\sim 80$  km). In addition to standard meteorological parameters (wind, temperature,  
127 moisture, surface pressure), this GCM includes 15 aerosol tracers (dust, sea-salt, sulfate, black  
128 and organic carbon), O<sub>3</sub> and CO<sub>2</sub>. The GEOS-5 NR is driven by prescribed sea-surface  
129 temperature and sea-ice, daily volcanic and biomass burning emissions, as well as high-  
130 resolution inventories of anthropogenic sources. A description of the GEOS-5 model  
131 configuration used for the Nature Run can be found in Putman et al. (2014), while results  
132 from a validation exercise appear in Gelaro et al. (2015) and Castellanos et al. (2019).

133 In a previous study of the MOD04\_DT code (Wind et al, 2016), we had the advantage of  
134 having simultaneous in situ aerosol property measurements from AEROSOL ROBOTIC NETWORK  
135 (AERONET) (Holben et al., 1998). AERONET has very limited data available over ocean,  
136 mainly from islands and ship transits. Even in places where AERONET is established, no  
137 measurements can be obtained in presence of clouds. Therefore, no ground-based in-situ  
138 measurements can be included in our analysis of the MOD06ACAERO product and so the  
139 analysis is necessarily limited to verification and closure.

140 In sections that follow we will describe the application of MCARS to study the  
141 MOD06ACAERO algorithm. Section 2 very briefly describes the MCARS code and the  
142 experiment setup. Section 3 describes the MODIS MOD06ACAERO product of Meyer et al.  
143 (2015). Section 4 shows the details of the study and study conclusions. Finally, section 5  
144 discusses the next steps in MCARS development.

## 145 **2 MCARS description**

146 The MCARS code was previously described in detail in Wind et al (2013, 2016).  
147 Therefore, only a brief description will be given here. Global aerosol, cloud, surface and  
148 atmospheric column fields from the G5NR simulation as described above serve as the starting  
149 point for radiance simulations. The GOCART bulk aerosol scheme currently used in the  
150 G5NR is used for the simulations reported in this paper, with corresponding optical properties  
151 as described in Randles et al. (2017), Hess et al (1998) and references within. The simulation  
152 input data was produced in accordance with the methods outlined in Wind et al. (2016). The  
153 G5NR model output was split into 1-km subcolumns (MODIS pixel resolution) using the  
154 independent column approximation method as described in detail in Wind et al. (2013). Here  
155 a brief summary of the model data preparation methodology is given.

156 MODIS pixels for each GEOS-5 gridbox were collected and the same number of pixel-  
157 like sub-columns was generated using a statistical model of sub-gridcolumn moisture  
158 variability. The sub-column generation used a parameterized probability density function  
159 (PDF) of total water content for each model layer and a Gaussian copula to correlate these  
160 PDFs in the vertical (Norris et al, 2008, Norris and da Silva 2016a,b).

161 The subcolumns generated in this way were subsequently rearranged, to give horizontal  
162 spatial coherence, by using a horizontal Gaussian copula applied to condensed water path.  
163 This arrangement had to be applied in order to create spatially coherent cloud-like structures.



164 The subcolumns themselves were not altered in any way during this process. If this step is  
165 skipped and the subcolumns are placed randomly within each gridbox the MODIS Cloud  
166 Optical and Microphysical Properties (MOD06) product (Platnick et al, 2017) would restore  
167 many of the pixels to clear sky unless the initial gridbox had close to 100% cloud fraction  
168 (Zhang and Platnick 2011; Pincus et al. 2012). The MOD06 product is a necessary input for  
169 MOD06ACAERO and must be produced prior to MOD06ACAERO execution. The need for  
170 this subcolumn rearrangement is significantly lessened when G5NR is used because the  
171 smaller gridboxes are often close to 100% cloudy especially in MBL regimes, but removing  
172 the method from the model preparation step was not practical due to its small impact on  
173 execution time and possibility of introducing errors.

174 The layer aerosol properties were obtained using the independent column approximation  
175 with the same PDF of total water content as used for clouds. A GEOS-5 aerosol species  
176 output file was used in conjunction with aerosol optical properties as in Randles et al. (2017).  
177 The aerosol phase functions for each of the 15 species output by GEOS-5 were produced and  
178 combined on the fly to create a single bulk set of scattering properties and Legendre  
179 coefficients. (Wind et al, 2016)

180 Model parameters such as profiles of temperature, pressure, ozone and water vapor  
181 together with layer information about clouds and aerosols are combined with solar and view  
182 geometry of the MODIS instrument. Surface information is also a combination of GEOS-5  
183 information of surface temperature, snow and sea ice cover and MODIS-derived spectral  
184 surface albedo (Moody et al. 2007, 2008). All of these parameters are transferred to the  
185 DISORT-5 radiative transfer code and reflectances and radiances in 22 MODIS channels  
186 between 470nm and 14.2 $\mu$ m are produced. The default computational resolution of DISORT-  
187 5 has also been increased to 32 streams up from 16 used in the two previous studies.  
188 Additionally some of the simulations in this study were executed at 64 streams. Final MCARS

189 output is packaged in a format identical to the standard MODIS Level-1B radiometric files  
190 and is thus completely transparent to any operational or research-level retrieval algorithm  
191 code.

192 These simulations were produced at the NASA Center for Climate Simulations (NCCS)  
193 supercomputer. Each complete simulation of a MODIS-like granule requires 5.5 hours of wall  
194 clock time on 300 processors. Computational throughput can be increased by limiting the  
195 scope of the simulation to fit a particular investigation. For this study, however, we retain the  
196 full set of channels needed for both cloud and aerosol research.

197

### 198 **3 MODIS above-cloud aerosol properties product**

199

200 The MODIS above-cloud aerosol properties product (MOD06ACAERO) (Meyer et al.  
201 2015) is a regional algorithm able to simultaneously retrieve MBL cloud optical thickness  
202 (COT), cloud effective radius, and aerosol optical depth (AOD) above-cloud in the SEAO  
203 region. It uses six MODIS channels (bands 1-5 and 7) having central wavelengths of 0.47,  
204 0.55, 0.66, 0.86, 1.24 and 2.1 $\mu\text{m}$ . The MOD06ACAERO algorithm takes advantage of the  
205 strong biomass burning aerosol absorption gradient in the visible (VIS) to near-infrared (NIR)  
206 spectrum that, when the aerosol layer overlies a bright cloud, yields differential attenuation  
207 (stronger at shorter wavelengths) of the otherwise nearly spectrally invariant top-of-  
208 atmosphere cloud reflectance across the VIS/NIR. Sensitivity to cloud optical thickness is  
209 localized in the spectral range between 0.47 and 1.24 $\mu\text{m}$  and is directly related to the  
210 magnitude of reflectance, while sensitivity to above-cloud aerosol optical depth is related to  
211 the spectral slope of the reflectance. The MOD06ACAERO algorithm uses 2.1 $\mu\text{m}$  channel for  
212 cloud effective radius information. That is also consistent with the principal retrieval  
213 contained in the MOD06 product (Platnick, et al, 2017)

214 The MOD06ACAERO retrieval inversion uses an optimal estimation-like approach  
215 (Rodgers, 1976) that attempts to minimize the difference (cost function) between the six  
216 MODIS reflectance observations and forward-modeled reflectance that is a function of cloud  
217 optical thickness, effective radius, and above-cloud AOD. However, rather than in-line  
218 radiative transfer calculations, MOD06ACAERO relies on a set of pre-computed lookup  
219 tables (LUTs) of coupled cloud and above-cloud aerosol reflectance. These LUTs are  
220 generated using the same cloud microphysics models used by MOD06 (Platnick et al, 2017)  
221 and the absorbing aerosol model used by MOD04\_DT over land surfaces (Levy et al, 2013).  
222 Retrievals using a second aerosol property model, one based on field campaign data from  
223 SAFARI 2000 (Haywood et al, 2003), are also available in MOD06ACAERO output. While  
224 these Haywood et al. model retrievals were recommended in Meyer et al (2015), evaluation  
225 during the ORACLES campaign revealed deficiencies at certain scattering angle ranges (K.  
226 Meyer, private communication). Thus, for this study we use the MOD06ACAERO results  
227 based on the MOD04\_DT aerosol models.

228 The MOD06ACAERO retrieval operates at 1km resolution, compared to the 10km and  
229 3km MOD04\_DT resolutions, and simultaneously provides pixel-level estimates of retrieval  
230 uncertainty accounting for known and quantifiable error sources (e.g., radiometry,  
231 atmospheric profile errors, cloud and aerosol forward model errors) consistent with the  
232 MOD06 cloud product methodology (Platnick et al, 2020). Figure 2 shows an example  
233 retrieval result from MOD06ACAERO compared to MOD04\_DT standard 10km output. The  
234 Terra MODIS granule shown here, from 2006 day 224 at 10:05 UTC, has extensive cloud  
235 cover over the ocean, typical for this season. MOD04\_DT provides a very limited amount of  
236 data, localized to the few areas of clear sky, while MOD06ACAERO fills in the above-cloud  
237 area. Shinozuka, et al (2020) suggest that above-cloud aerosol retrievals are similar to  
238 adjacent clear-sky retrievals and so clear-sky retrievals could be used as an above-cloud

239 proxy. However conditions shown in Figure 2 are common during the SEAO burning season.  
240 There are no clear-sky retrievals of aerosol over most of the area due to near uniform  
241 coverage by marine stratus, with cloud fraction approaching 80%. Nearest successful clear-  
242 sky retrievals are hundreds of miles away. Therefore an above-cloud aerosol retrieval  
243 algorithm such as MOD06ACAERO is very much so necessary.

244 MOD06ACAERO uses National Center for Environmental Prediction (NCEP)  
245 atmospheric profile products (Derber et al, 1991) for atmospheric correction. As part of our  
246 investigation we will look at impact of discrepancies between NCEP and G5NR on retrieved  
247 aerosol properties.

248

#### 249 **4 Analysis**

250

251 To create the data used for the MOD06ACAERO verification study, we examined the  
252 G5NR dataset for cases that were similar to conditions commonly encountered during the  
253 burning season over SEAO. August 2006 was selected because it was a very active smoke  
254 season and a significant amount of MBL clouds were present in the model output. Models  
255 often have difficulties forming MBL clouds as higher than usual grid and vertical resolution is  
256 needed in order to accurately represent the processes that lead to MBL formation in nature.

257 As real Terra and Aqua overpasses are needed in order to define the sun-satellite  
258 geometry for the MCARS simulations, satellite orbital tracks had to be considered. Because  
259 orbital gaps are prominent in the MODIS data over the SEAO MBL region, care must be  
260 taken in selecting specific days and times having adequate sensor geometry. Technically  
261 because MCARS is a simulation, orbital gaps have no meaning. But because of the need of  
262 actual sensor geometry to start the simulation, it is most expedient to simply browse available  
263 MODIS data for a suitable track. Even though G5NR does not perform any data assimilation,

264 the model code is identical to the standard GEOS-5 model. MCARS normally runs on  
265 standard GEOS-5 output. In Wind et al (2013) we showed MCARS as a model output  
266 verification tool. It is always very desirable to match date/time/orbit when model performance  
267 may be compared to real concurrent sensor measurements. Even though no orbital match is  
268 required in this study, a decision was made to not alter the standard MCARS operation in  
269 order to avoid accidental introduction of software issues. Five cases were selected under these  
270 considerations. Three came from Terra MODIS overpasses and two from Aqua MODIS. The  
271 times and dates were as follows. Terra MODIS: 2006 day 224, 10:05 UTC, 2006 day 225  
272 09:10 UTC, 2006 day 228 09:40 UTC. Aqua MODIS: 2006 day 224 12:55 UTC and 2006 day  
273 226 12:40 UTC. This simulated radiance dataset comprises 13.5 million points where the  
274 atmospheric column and surface conditions are explicitly known. MOD06ACAERO retrievals  
275 were attempted over those points, but of course that does not mean that each attempt produced  
276 a successful aerosol retrieval.

277 Figure 3 a) shows simulated RGB images for the 5 MCARS MODIS granules listed  
278 above. Also shown in b) are the same simulated granules where the aerosols have been  
279 removed from the radiative transfer simulations. This ability to remove clouds, aerosols or  
280 gases from the simulation offers extensive control evaluating the performance of retrieval  
281 algorithms and diagnosing algorithm deficiencies.

282 There is a significant similarity between the real Terra MODIS granule of Figure 2 and  
283 the simulated granule for the same date and time. The G5NR is a free running model and does  
284 not perform any data assimilation, and therefore it is not synoptically locked to the particular  
285 day depicted in Figure 2. The apparent similarities between Figures 2 and 3 merely reflect the  
286 persistent patterns of MBL clouds and smoke in the region. There is no expectation of a match  
287 with any real data in this study. It is not a statement to G5NR performance as in other cases  
288 the cloud amount/distribution had no match to any real data. It is merely an interesting

289 coincidence. Some granules were selected to include a significant portion of land surface for a  
290 later examination of the MOD04\_DT retrievals, repeating the study in Wind et al (2016) in a  
291 different region (not reported here).

292 This dataset, both the complete and the clean (aerosol-free) versions, was fed through the  
293 standard operational MODIS Data Collection 6 cloud product processing chain to produce  
294 cloud mask, MOD06 cloud top and optical properties, and finally the MOD06ACAERO  
295 output for each case. Results from all granules were then combined and only retrievals for  
296 cloudy pixels were examined. The MOD06ACAERO aerosol retrievals were compared to  
297 source aerosol optical depth provided by GEOS-5 (Wind et al, 2016). Figure 4 shows results  
298 of this comparison. The only constraint on this comparison was that the algorithm-reported  
299 pixel-level retrieval uncertainty had to be less than 40% for panel a) and less than 30% for  
300 panel b). One of the motivations of this study was to characterize errors in the  
301 MOD06ACAERO algorithm for subsequent aerosol data assimilation into GEOS-5. Pixels  
302 with higher uncertainties could be considered in the analysis, but assimilating data where the  
303 retrieval error is 50% or greater could negatively impact the assimilated fields. As depicted in  
304 Figure 4, filtering retrievals at the reported algorithm uncertainty at 40% is very effective to  
305 produce a good match between MOD06ACAERO and the G5NR output variables, with the  
306 exception of very low AODs. G5NR uses aerosol models described in detail in Randles et al  
307 (2017). It is a set of 15 absorbers, properties of which are a function of column relative  
308 humidity. MOD06ACAERO in this study uses the MOD04\_DT aerosol models, which are  
309 distinct in composition and additionally computed at a constant 80% column relative humidity  
310 (Levy et al, 2013). Because G5NR mixes aerosols on-the-fly to create bulk layer properties  
311 and MOD06ACAERO has a constant regional mixture, there is a natural source of uncertainty  
312 in any comparison of MOD06ACAERO retrievals with G5NR. However the regional mixture  
313 of MOD04\_DT had been used extensively to train the GOCART model used by both GEOS-5

314 and G5NR. Thus we expect the uncertainty due to aerosol model mismatch to be fairly  
315 minimal. Same exact situation of aerosol mixture mismatch exists in real data and is most  
316 likely greater than the one existing in this simulation. Detailed comparison of GOCART and  
317 MOD04\_DT aerosol models for biomass burning aerosols has been performed in Wind et al  
318 (2016).

319 Meyer et al. (2015) suggest that additionally MOD06ACAERO retrievals should be  
320 screened by retrieved cloud optical thickness and that they should be discarded if COT is less  
321 than 4.0. We applied this additional constraint onto the retrieval comparison and the result is  
322 shown in Figure 5. Discarding the AOD retrievals when cloud is thin improved the match-up  
323 against GEOS-5, but there still appears to be an issue when GEOS-5 AOD is very close to  
324 zero.

325 The power of MCARS lies in being able to tightly control simulation parameters. The  
326 MOD06ACAERO algorithm appears to run into a difficulty at low source AOD. In order to  
327 examine the causes for this discrepancy in more detail, we turn our attention to the clean  
328 MCARS case shown in figure 3b) by setting the AOD precisely to zero and examining the  
329 retrieval performance in such situation. Ideally MOD06ACAERO should retrieve a zero AOD  
330 throughout. With an exception of a narrow range of scattering angles between 135 and 145  
331 degrees, which corresponds to the cloud bow direction, the algorithm indeed retrieved AOD  
332 that was extremely close to zero. Figure 6 depicts the difference between retrieval and source  
333 as a function of scattering angle. Retrievals where MOD06ACAERO matched GEOS-5  
334 precisely were discarded for clarity. Within the cloud bow MOD06ACAERO tends to return a  
335 small positive AOD of about 0.15.

336 The liquid water phase function is very complex in the cloudbow region and is very  
337 difficult to model accurately. That particular region has consistently caused difficulties to the  
338 standard MOD06 product retrievals of MBL clouds. Both MOD06 and MOD06ACAERO

339 LUTs are computed at 64 DISORT streams. We performed some investigation of this area by  
340 running a special simulation for a single case from Terra 2006 day 224 10:05 UTC. This case  
341 was selected because the cloudbow is especially noticeable in both real and simulated data.  
342 The simulation was also executed using 64 DISORT streams in order to reduce uncertainties  
343 associated with the simulation being performed at half the resolution. In cloudbow region  
344 more streams would potentially lead to a better model. Unfortunately the cloudbow persisted.  
345 It thus may be the case that 64 streams are not sufficient to properly resolve the cloudbow in  
346 either simulation or retrieval. Even higher resolution may be advisable. Increasing  
347 computational resolution of MOD06 LUTs is presently considered for the upcoming MODIS  
348 Data Collection 7. Depending on the results, same increase may occur for MOD06ACAERO.  
349 At this time, for purpose of establishment of assimilation constraints, which is the focus of  
350 this study, one might simply exclude the cloud bow scattering angle range from consideration  
351 until more is known.

352 Figure 7 shows the results of MOD06ACAERO retrievals from Figure 5 where retrievals  
353 within the cloud bow have been discarded. The comparison with source data is further  
354 improved and the cluster of MOD06ACAERO retrievals present in Figure 5 when GEOS-5  
355 AOD was near zero has disappeared.

356 Often better retrievals can be obtained when less oblique view geometry is considered in  
357 real data. Pixel size, longer optical path length and 3D effects from clouds can all make  
358 retrievals performed at oblique view angles less optimal. In the case of this study, another  
359 consideration for imposition of a view zenith limit is that presently MCARS does not account  
360 for pixel size growth at oblique view angles. The number of subcolumns generated does not  
361 change with view zenith angle. Therefore, MCARS results when view angle is oblique may  
362 not be an accurate measure of algorithm performance as only the effects of optical path length  
363 are simulated.



364 The MOD06 cloud product outputs cloud top pressure, temperature and height limited to  
365 near nadir in addition to full swath products. The “near nadir” is defined as viewing zenith  
366 angle less than 32 degrees (Menzel et al, 2008). Figure 8 shows the MOD06ACAERO  
367 retrievals of Figure 7 further limited by view zenith angle of less than 32 degrees. When view  
368 zenith angle is limited to 32 degrees the comparison with GEOS-5 source data is again  
369 improved. We can now show a slope of 0.866 for retrievals with less than 40% error and  
370 0.913 for retrievals with error of less than 30%. Note that even though the data extent had  
371 been limited, there are still over 600,000 data points left to be ingested into a model if data  
372 assimilation were to be attempted in an area where previously the number of such data points  
373 was close to 0.

374 We can constrain the view zenith angle range even further as shown in Figure 9, reducing  
375 the threshold to 20 degrees. Whereas the comparison shows all around improvement with  
376 slope of 0.931 and 0.977 for retrieval error of less than 40% and 30% respectively, the number  
377 of points suitable for assimilation shrinks by half. It is not clear if this dataset size reduction  
378 can be justified by the improvement in alignment with the source data.

379 With the 20 degree view angle constraint the algorithm results are very close to source  
380 data and we could potentially state that we have closure against source GEOS-5 data even  
381 though both MOD06 and MOD06ACAERO run under operational conditions used NCEP  
382 GDAS data for atmospheric correction (implying a likely overestimation of the error in these  
383 profiles). In order to assess the impact of using these GDAS-based profiles we consider a final  
384 experiment where we use MCARS pixel-level input profiles for atmospheric correction. The  
385 result is shown in Figure 10. When atmospheric profiles are removed as a source of  
386 inconsistency, the agreement with source data improves to a slope of 0.996 with intercept of -  
387 0.007 and RMSE of 0.097 for retrievals with less than 40% error and slope of 0.989, intercept  
388 of 0.03 and RMSE of 0.085 for retrievals with less than 30% error. Small sample size for

389 retrievals with lower uncertainty is the reason for somewhat lesser agreement with source data  
390 for this closure experiment. The remaining source of potential disagreement of  
391 MOD06ACAERO retrieval with input GEOS-5 data is the difference between aerosol models  
392 used by MCARS and MOD06ACAERO. Cloud models between MOD06ACAERO and  
393 MCARS are identical in this study. The MOD06ACAERO model is fixed for the region,  
394 while the GEOS-5 aerosols are fully dynamic as per Randles et al (2017). However, it is not  
395 practical to change either MCARS or MOD06ACAERO code to use a different aerosol model  
396 set, and with the agreement being as good as it presently is.

397

## 398 **5 Conclusions and future directions**

399 This paper is a direct evolution of work started in Wind et al, (2013) and continued in  
400 Wind et al (2016). The Multi-sensor Cloud and Aerosol Retrieval Simulator (MCARS) has  
401 now been applied as a verification tool for a research-level algorithm. The algorithm studied  
402 was the MODIS above-cloud aerosol properties retrieval algorithm of Meyer et al (2015).  
403 MCARS computational resolution has been doubled and for this study the high-resolution  
404 (7km) GEOS-5 Nature Run model was utilized. The MCARS code produces radiances and  
405 reflectances in a standard MODIS Level 1B format after sending the GEOS-5 data through  
406 DISORT-5 radiative transfer code. The output can be directly ingested by any retrieval or  
407 analysis code that reads data from the MODIS instrument.

408 We used the MCARS code to perform verification and closure study on the  
409 MOD06ACAERO algorithm. In this study we generated a set of five MODIS granules located  
410 in the Southeastern Atlantic Ocean off the coast of Namibia. We executed the  
411 MOD06ACAERO code on this case set. In the verification part of the study the algorithm  
412 performed very well. When pixels with less than 30% uncertainty were considered with  
413 underlying cloud layer having optical thickness greater than 4 the algorithm matched the

414 source GEOS-5 aerosol optical depth with slope of 0.774 and offset of 0.076, RMSE = 0.131.  
415 On further examination, executing the algorithm on the same case set with aerosols removed it  
416 was determined that there might be data that is less useful around the scattering angle of 140  
417 degrees, the cloud bow direction. When the cloud bow pixels were excluded the slope  
418 improved to 0.913. The near-nadir slope with angle limit of 20 degrees improved the  
419 agreement further to 0.977, RMSE=0.096.

420 To look at closure one of the five cases was selected. For closure both MOD06 and  
421 MOD06ACAERO codes were modified to use MCARS input profiles as ancillary instead of  
422 the NCEP analysis used in operations (Platnick et al, 2017). When the results were compared  
423 to source GEOS-5 data a slope of 0.996 with offset of -0.007 and RMSE = 0.097 was reached  
424 for pixels with less than 40% uncertainty. The agreement was slightly worse for uncertainties  
425 less than 30% (slope 0.989, offset 0.03 and RMSE = 0.085) but that was mainly due to having  
426 a smaller number of pixels in the set, only 130,000.

427 The results of this study suggest that retrievals produced by MOD06ACAERO are of  
428 good initial quality and would be a valuable addition to model data assimilation streams with  
429 the following constraints. MOD06ACAERO pixels should be assimilated if retrieval  
430 uncertainty is less than 40%, if optical thickness of the underlying cloud layer is greater than  
431 4.0 and if the pixel scattering angle is outside the cloud bow. Additionally, an even tighter  
432 constraint can be added to only take pixels that are near nadir.

433 This study is yet another example of the capabilities of the MCARS framework. There  
434 are many other potential applications of the MCARS code, including extending the simulator  
435 to other sensors and examining the performance of fast retrieval simulators used in climate  
436 modeling.

## 437 **6 Code and Data Availability**

438 The MCARS code is free of charge and can be downloaded here:

439 [https://zenodo.org/record/5224964#.YR\\_DOdNKjaV](https://zenodo.org/record/5224964#.YR_DOdNKjaV)

440

441

442

443 **Author Contributions**

444 GW is the development and experiment design lead on the MCARS project. She  
445 maintains the code, creates experiments and performs most of the analysis of experiment data.

446 AdS and PN assist with preparation, interpretation and integration of the GEOS-5 model  
447 data.

448 KM is the author of MODIS above-cloud aerosol retrieval algorithm, the subject of this  
449 simulation experiment. He assisted with interpretation of retrieval results and development of  
450 assimilation constraints for the above-cloud aerosol product.

451 SP assisted with analysis, evaluation and interpretation of all experiment data.

452

453 **Acknowledgements**

454 The authors would like to thank Brad Wind for the initial idea for creating a simulator,  
455 the output of which could be transparently used with remote sensing retrieval codes.

456

457



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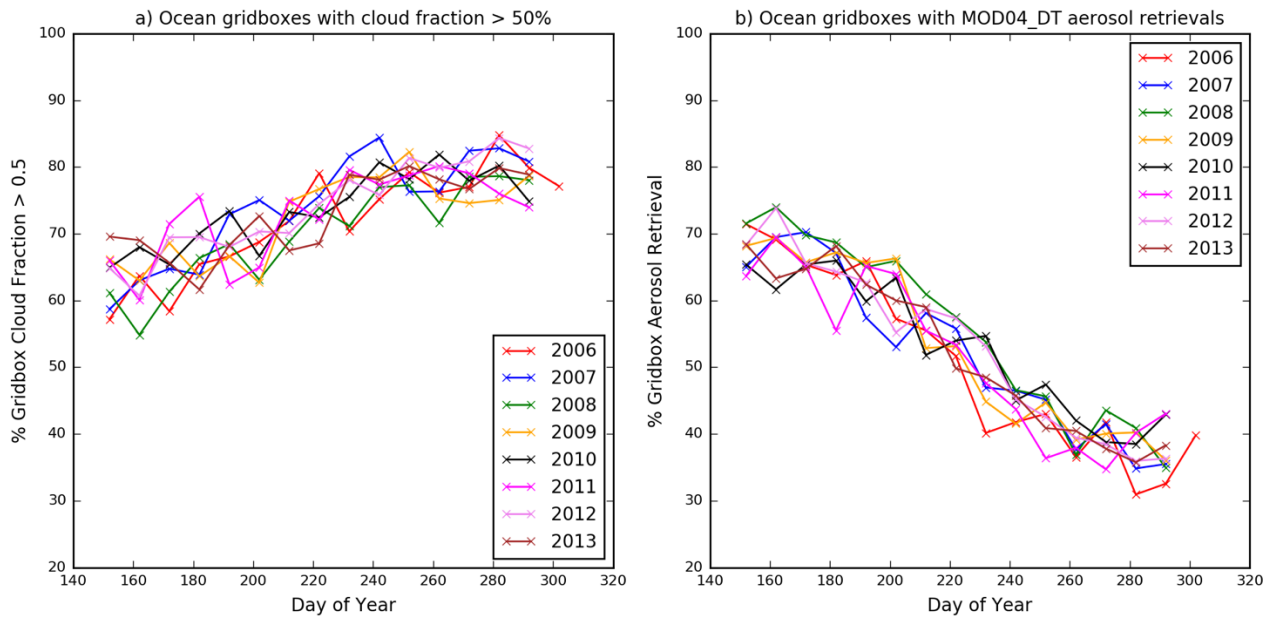
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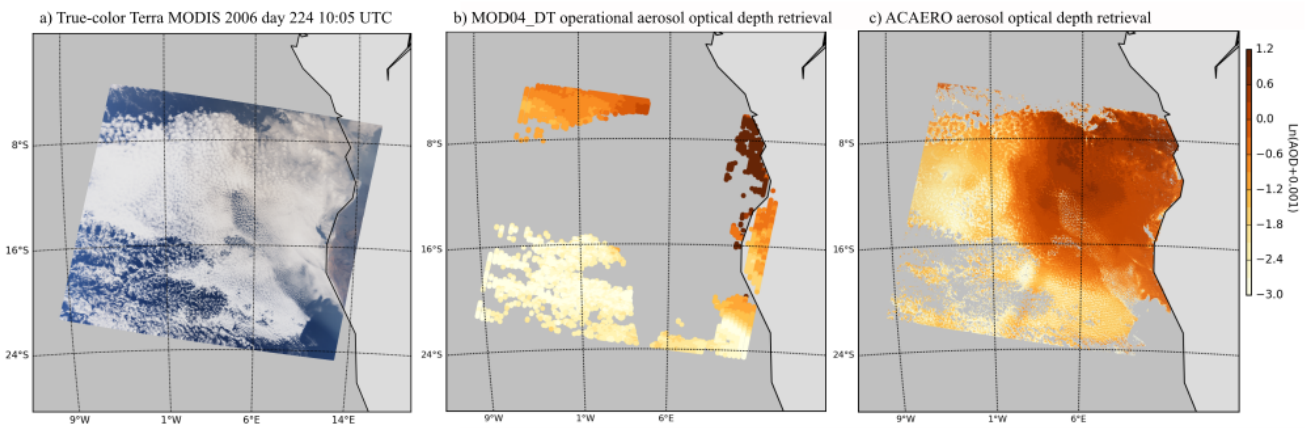
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Figure 1. Terra MODIS Level-3 Daily 1-degree gridded product for SEAO area for years 2006-2013. Panel a) shows the percentage of SEAO ocean gridboxes that had cloud fraction greater than 50%. Panel b) shows the percentage of SEAO ocean gridboxes that had any successful MOD04DT aerosol property retrievals of any quality.

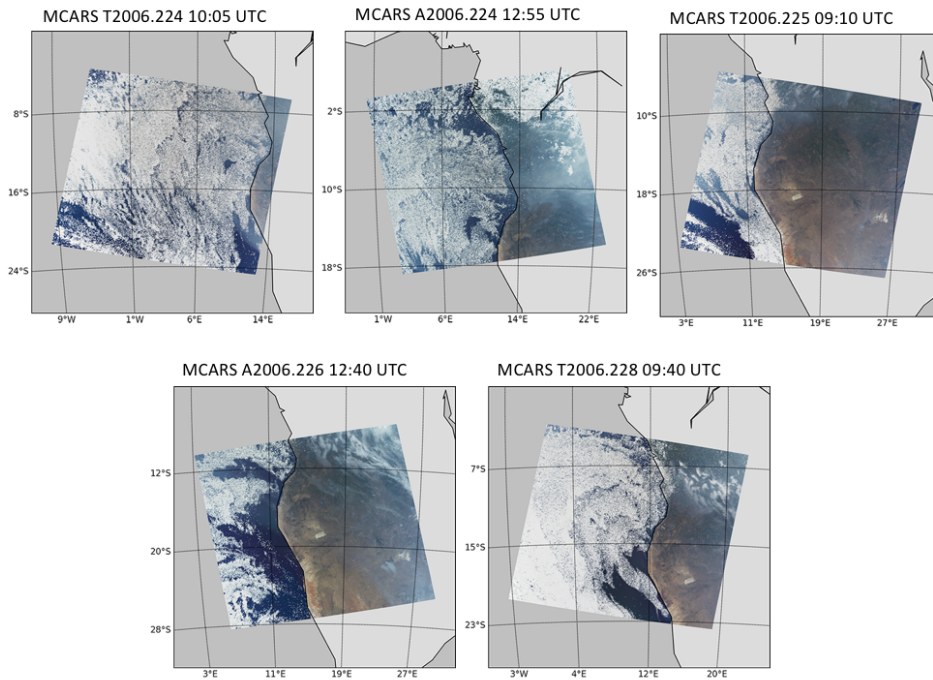
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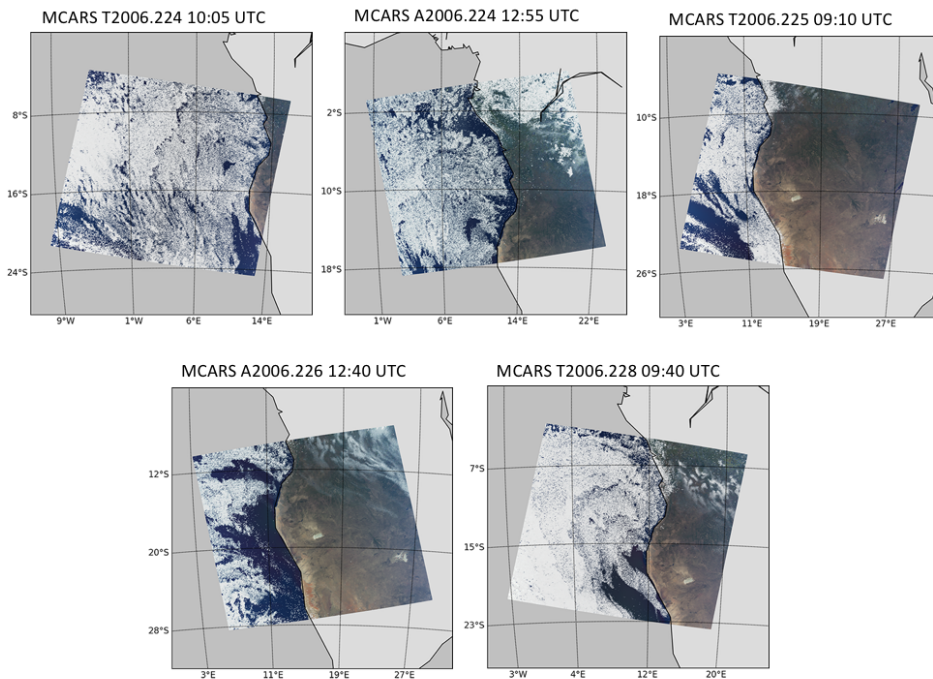
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Figure 2. Real-data example of MOD06ACAERO retrieval. Terra MODIS 2006 day 224 10:05 UTC. Panel a) shows the true-color MODIS granule. There is extensive aerosol layer above the equally extensive MBL cloud layer. Panel b) shows the MODIS Data Collection 6 operational Dark Target aerosol retrieval. It is a 10km resolution product with retrievals available only in clear sky conditions and outside glint. Panel c) shows the MOD06ACAERO above-cloud aerosol retrieval that is able to fill the data gap created by presence of MBL layer.

a) MCARS study cases with aerosols included

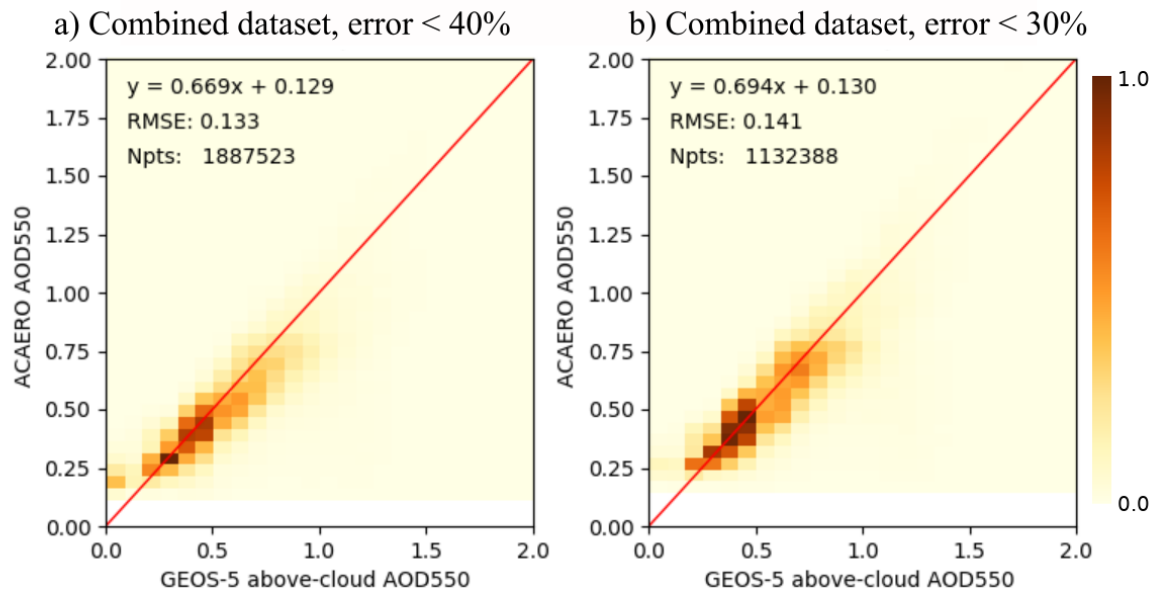


b) MCARS study cases with aerosols removed



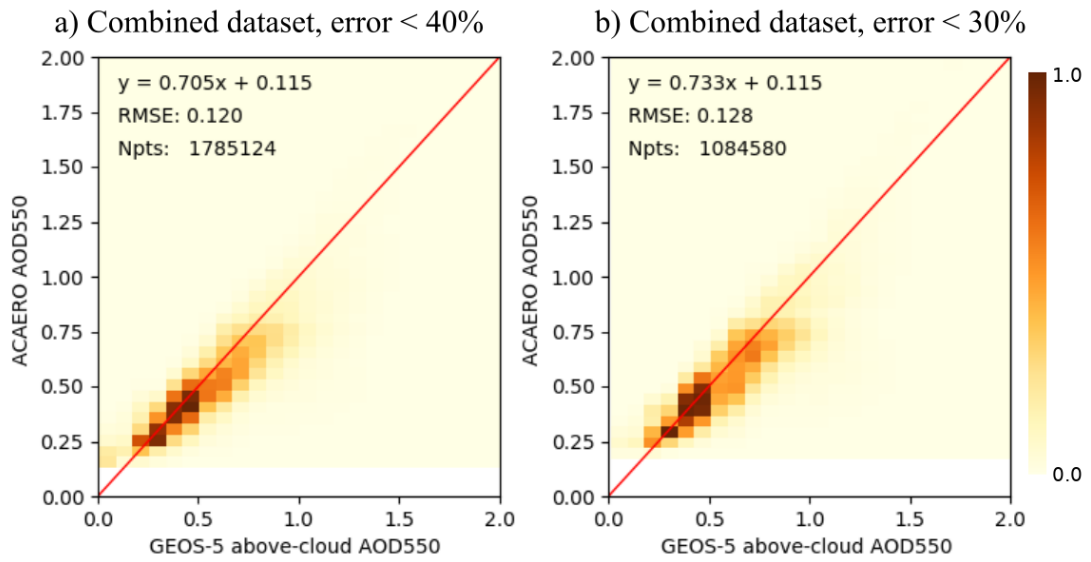
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Figure 3. Scenes generated by MCARS from G5NR used in analysis of the MOD06ACAERO product. There are three cases based on Terra MODIS, designated with a T next to the year. There are two cases based on Aqua MODIS, designated with an A next to the year. Panel a) shows the case set simulated with aerosols present. Panel b) shows the same case set but simulated with aerosols removed.



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 666 Figure 4. MOD06ACAERO retrieval results from the combined dataset of Figure 3a  
 667 compared to source GEOS-5 aerosol optical depth as a normalized density plot. No screening  
 668 of retrievals had been performed except for pixel-level uncertainty. Panel a) shows  
 669 MOD06ACAERO retrievals with uncertainty of less than 40% and panel b) shows same with  
 670 uncertainty less than 30%.  
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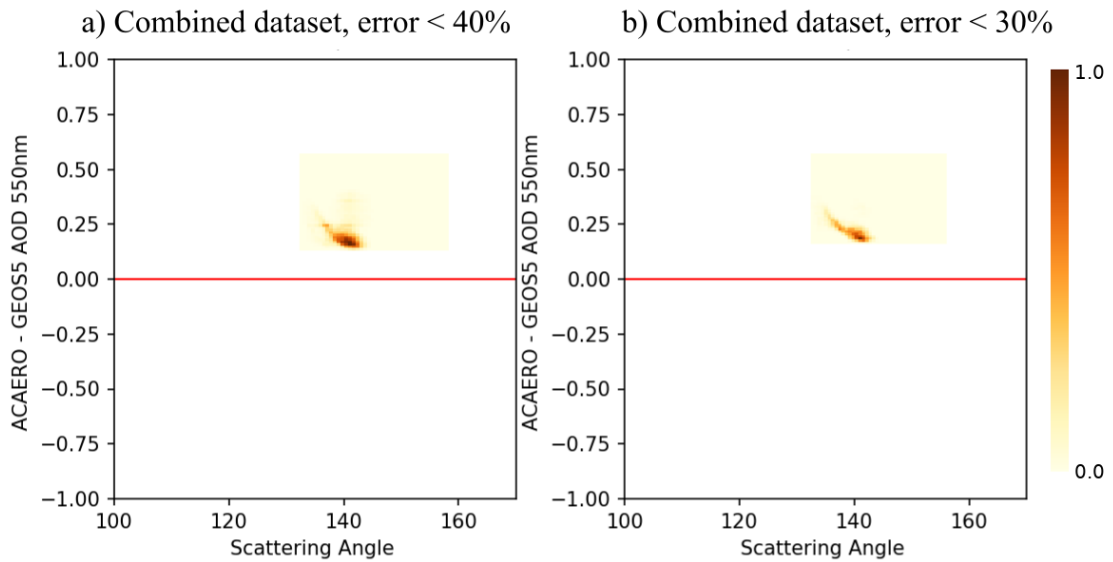




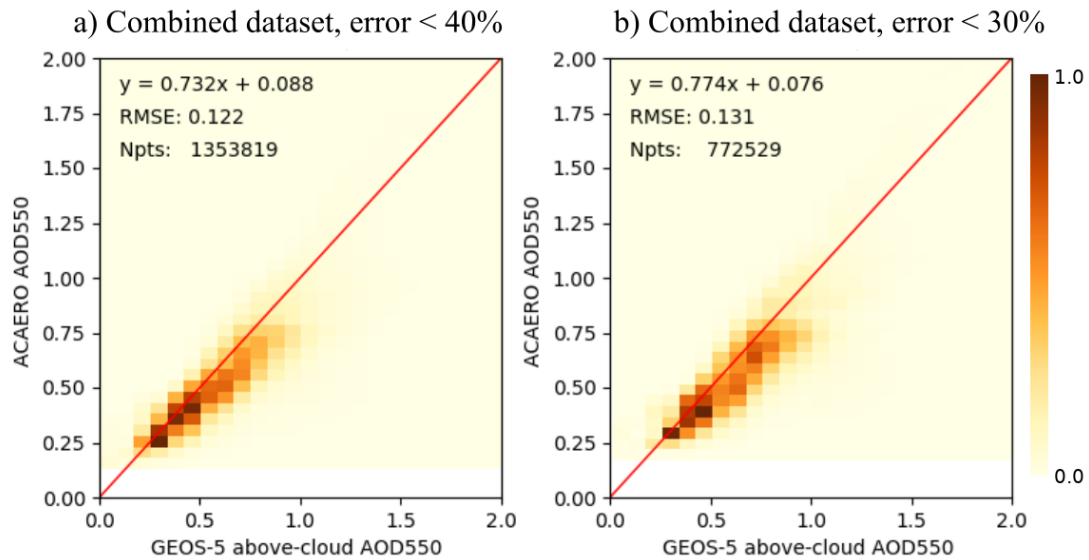
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Figure 5. MOD06ACAERO retrieval results from the combined dataset of Figure 3a compared to source GEOS-5 aerosol optical depth as a normalized density plot. AOD retrievals where COT was less than 4 are now discarded. Panel a) shows MOD06ACAERO retrievals with uncertainty of less than 40% and panel b) shows same with uncertainty less than 30%.

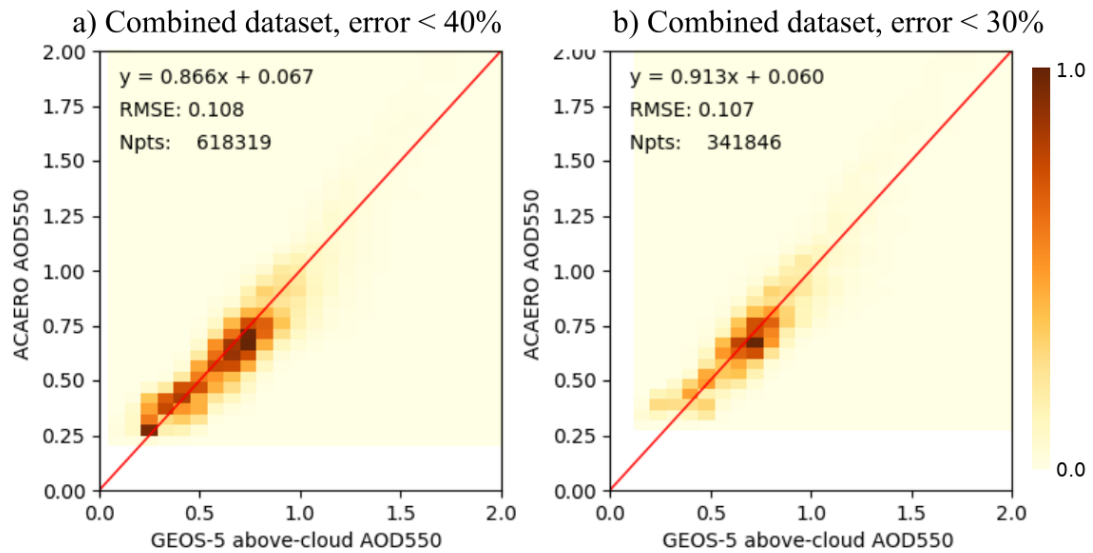




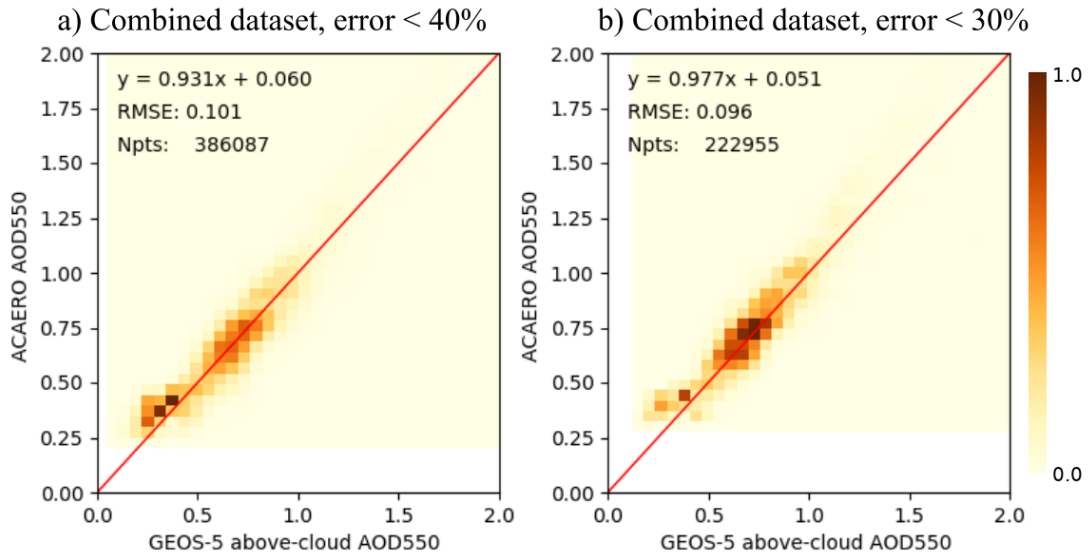
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 681 Figure 6. MOD06ACAERO retrieval results from the combined dataset of Figure 3b, where  
 682 aerosols had been removed. The results are displayed as difference from GEOS-5 AOD,  
 683 which in this case was zero, as a function of scattering angle as a normalized density plot. All  
 684 retrievals where MOD06ACAERO result was also zero had been removed for clarity. All  
 685 non-zero MOD06ACAERO retrievals appear to be concentrated in a narrow angle range  
 686 between 135 and 145 degrees which corresponds to the cloud bow. Panel a) shows  
 687 MOD06ACAERO retrievals with uncertainty of less than 40% and panel b) shows same with  
 688 uncertainty less than 30%.  
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 692 Figure 7. MOD06ACAERO retrieval results from the combined dataset of Figure 3a  
 693 compared to source GEOS-5 aerosol optical depth as a normalized density plot. AOD  
 694 retrievals where COT was less than 4 are now discarded. Additionally retrievals in the cloud  
 695 bow region are also removed. It appears they were indeed the source of a cluster of higher  
 696 MOD06ACAERO retrievals when GEOS-5 AOD was near zero and the match up with  
 697 GEOS-5 source AOD is further improved. Panel a) shows MOD06ACAERO retrievals with  
 698 uncertainty of less than 40% and panel b) shows same with uncertainty less than 30%.  
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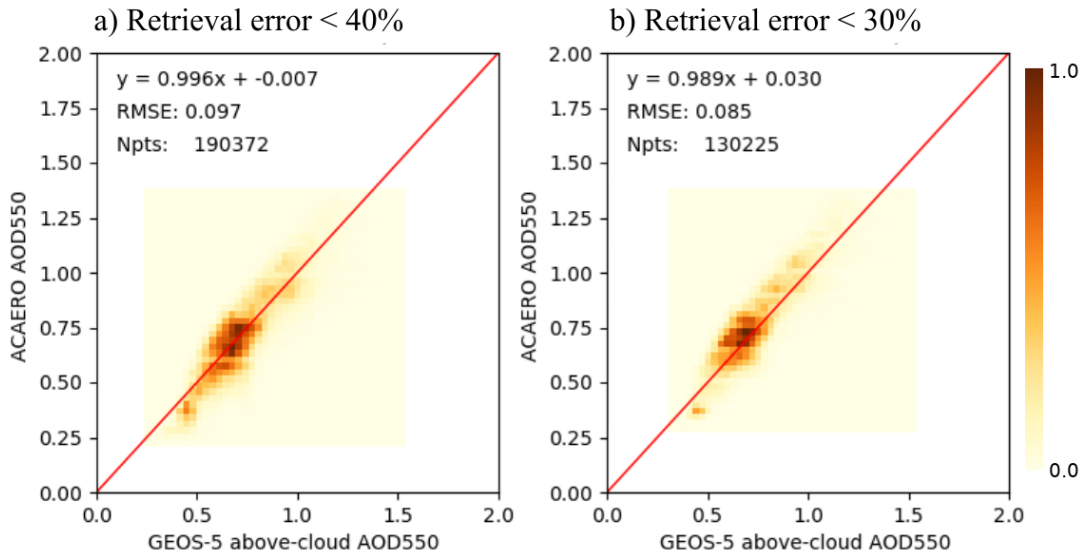
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 702 Figure 8. MOD06ACAERO retrieval results from the combined dataset of Figure 3a  
 703 compared to source GEOS-5 aerosol optical depth as a normalized density plot. AOD  
 704 retrievals where COT was less than 4 and where the scattering angle was in the cloud bow are  
 705 now discarded. Additionally the data extent had been limited to only include pixels with view  
 706 zenith angle of less than 32 degrees. Retrieval comparison shows further improvement. Panel  
 707 a) shows MOD06ACAERO retrievals with uncertainty of less than 40% and panel b) shows  
 708 same with uncertainty less than 30%.



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Figure 9. MOD06ACAERO retrieval results from the combined dataset of Figure 3a compared to source GEOS-5 aerosol optical depth as a normalized density plot. AOD retrievals where COT was less than 4 and where the scattering angle was in the cloud bow are now discarded. Additionally the data extent had been limited to only include pixels with view zenith angle of less than 20 degrees. Retrieval comparison shows further improvement however it is not clear if the reduction in dataset size is worth the gain in accuracy. Panel a) shows MOD06ACAERO retrievals with uncertainty of less than 40% and panel b) shows same with uncertainty less than 30%.

### MCARS Terra MODIS 2006 day 224, 10:05 UTC



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Figure 10. MOD06ACAERO retrieval results from simulated MCARS granule based on Terra MODIS 2006 day 224 10:05 UTC compared to source GEOS-5 aerosol optical depth as a normalized density plot. In this experiment both MOD06 and MOD06ACAERO were modified to use MCARS pixel-level atmospheric profiles to perform atmospheric correction. AOD retrievals where COT was less than 4 and where the scattering angle was in the cloud bow are now discarded. Additionally the data extent had been limited to only include pixels with view zenith angle of less than 20 degrees. This experiment shows excellent agreement with source data. Panel a) shows MOD06ACAERO retrievals with uncertainty of less than 40% and panel b) shows same with uncertainty less than 30%. The small dataset size in panel b) is the reason for slightly lower agreement with source compared to panel a)