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Multi-sensor cloud and aerosol retrieval simulator and remote sensing from model parameters – Part 2: Aerosols

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Abstract

The Multi-sensor Cloud Retrieval Simulator (MCRS) produces synthetic radiance data from model output as if a specific sensor such as the Moderate Resolution Imaging Spectroradiometer (MODIS) were viewing an atmospheric column. Previously the MCRS code only included contributions from atmosphere and clouds in its radiance calculations and did not incorporate properties of aerosols. In this paper we added a new aerosol properties module to the MCRS code that allows user to insert a mixture of up to 15 different aerosol species in any of the 36 available simulated layers.

The MCRS code is currently known as MCARS (Multi-sensor Cloud and Aerosol Retrieval Simulator). Inclusion of an aerosol module into MCARS not only allows for extensive, tightly controlled testing of various aspects of satellite operational cloud and aerosol properties retrieval algorithms; but also provides a platform for comparing cloud and aerosol models against satellite measurements. This kind of two-way platform can improve the efficacy of model parameterizations of measured satellite radiances, thus potentially improving model skill.

The MCARS code provides dynamic controls for appearance of cloud and aerosol layers. Thereby detailed quantitative studies of impacts of various atmospheric components can be conducted in a controlled fashion. The aerosol properties used in MCARS are directly ingested from GEOS-5 model output. They are prepared using the same model subgrid variability management methods as are used for cloud and atmospheric properties profiles, namely the Independent Column Approximation (ICA) technique. After MCRS computes sensor radiances equivalent to their observed counterparts, these radiances are substituted into an operational remote sensing algorithm.

Specifically, the MCRS computed radiances are input into the processing chain used to produce the MODIS Data Collection 6 aerosol product (M{O/Y}D04) that would normally be

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produced from actual sensor output.

We show direct application of this synthetic product in analysis of performance of the MOD04 operational algorithm. We use biomass burning case studies employed in a recent Working Group on Numerical Experimentation (WGNE) -sponsored study of aerosol impacts on Numerical Weather Prediction (Freitas et al. 2016). We show that a known low bias in retrieved MODIS aerosol optical depth appears to be due to a disconnect between actual column relative humidity and the value assumed by the MODIS aerosol product.

1 Introduction

Aerosols in the atmospheric column are a significant source of uncertainty for passive remote-sensing (e.g. from a satellite) retrievals of cloud optical and microphysical properties. Thick aerosol layers can be wrongly identified as clouds, and aerosols above clouds will lead to biases in cloud retrievals (Meyer et al. 2013). Biases in cloud detection and retrievals of cloud microphysics will lead to uncertainties in properties important for quantifying Earth's radiative budget. On the other hand, clouds wrongly identified and retrieved as aerosol may have similar impacts on estimates of aerosol radiative forcing and effects on climate and clouds. The Moderate-resolution Imaging Spectrometer (MODIS; Barnes et al. 1998) has been flying on the polar orbiting (at 705 km altitude) satellites known as Terra (since 2000) and Aqua (since 2002). Viewing a 2300 km swath, split into 5-minute granules, MODIS measures radiance (or reflectance) in 36 spectral channels, for which 19 are in reflective solar bands, with the other 17 being terrestrial emission. All bands are in at least 1 km spatial resolution. Based on MODIS observations, separate teams have created high-quality retrievals of both cloud (e.g. the M{O/Y}D06_L2 (MxD06); Platnick et al, 2003) and aerosol (M{O/Y}D04_L2 (MxD04; Levy et al., 2013) products. Current operational cloud retrieval includes methods for clearing the aerosols mis-identified as clouds from retrieval attempts. (Zhang and Platnick 2011; Pincus et al. 2012). Similarly for aerosol retrievals, much effort is made to reclassify as "not cloudy" scenes that are in fact, heavy dust or smoke. Therefore, for both teams, uncertainty whether a particular sample is cloud-covered or contains primarily aerosols, and how to propagate this uncertainty into retrieval products, remains a topic of great interest. A major problem is that there is no absolute ground-truth to confirm or deny these decisions in all cases. Ground based instrumentation such as sun photometers (Holben et al 1998) may not be able to accurately distinguish between aerosol and thin clouds due to limited spectral range, reaching only up to 1.024µm. There are also efforts to retrieve aerosol optical depth above cloud layers (Meyer and Platnick 2015, Meyer et al. 2013). Validation for such algorithms is often done using lidar and radar data. (Notarnicola, et al. 2011, Ackerman, et al. 2008) However as current spaceborne lidar and radar instruments do not scan, the amount of such data acquired in tandem with an instrument like MODIS is rather limited.

While a global meteorological model cannot be directly used to validate observations and retrievals due to the many assumptions and simplifications commonly made when such models are created (Rienecker et al. 2008), one could use such a model to learn about sensitivities of retrieval algorithms. As global models such as the Goddard Earth Observing System Model, Version 5 (GEOS-5; Rienecker et al. 2008, Molod et al. 2012), become increasingly realistic when simulating aerosols and clouds over complex surface terrain, we can apply detailed radiative transfer (RT) to simulate how these scenes would appear to a satellite such as MODIS, and how operational algorithms would in turn retrieve the specified conditions. Since the specified model aerosol and cloud properties of the scene are known, one can then characterize the ability (and uncertainties) of standard (e.g. MxD04 or MxD06) retrievals in these scenes. Thus, one can evaluate the current (and possibly historical) performance of cloud and aerosol properties retrievals. Application and evaluation of these simulation capabilities for known instruments is also an important step in development of Observing System Simulation Experiments for future observing missions.

The Multi-Sensor Cloud and Aerosol Retrieval Simulator (MCARS; Wind et al., 2013) is a modular, flexible tool, in which model output is coupled with a radiative transfer code in order to simulate Top Of Atmosphere (TOA) radiances that may be measured by a remote sensing instrument if it were passing over the model fields. In principle, MCARS can be used with any model and any sensor. The simulation complexity is only limited by computer power. However, in this paper, the MCARS continues to use the combination of GEOS-5

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model and Discrete Ordinate Radiative Transfer (DISORT) code (Stamnes et al. 1988) to simulate MODIS radiances. In Wind et al. (2013), the MCARS simulated only clouds; here we add microphysical properties of aerosols present in scenes we examine.

The approach we take is to populate the operational MODIS Level 1B calibrated radiance files with TOA radiances simulated from GEOS-5 model output and DISORT. For a given time and location, MODIS provides a particular geometry of observation. Since GEOS-5 includes outputs of clouds and aerosols above a surface, we can replace the MODIS-observed reflectance data with simulations. Then we run the standard aerosol (MxD04_L2) and cloud (MxD06_L2) retrieval codes and compare retrieval result to the known GEOS-5 source data. The discrepancies diagnosed by this device can then be contrasted to discrepancies obtained by comparing the real operational retrievals to independent, trusted observations (e.g., AOD from AERONET). To the extent that simulated and real statistical comparisons match, we can use capabilities of the MCARS code to examine the causes for such discrepancies, and hopefully identify opportunities for algorithm improvement. Since the aerosol retrieval is under-determined (Levy et al. 2013) and a number of assumptions must be made, the MCARS simulation approach is highly valuable as individual assumptions can be tested in isolation. The MCARS code has sufficient flexibility to test impacts of settings of single operational retrieval code parameters without interference from other components.

In sections that follow we will describe the improved MCARS system. Section 2 describes the GEOS-5 aerosol properties and their addition into MCARS. Section 3 describes the MODIS aerosol product. Section 4 discusses case selection for the current analysis. It shows the selected scenes simulated by MCARS and describes other special simulation settings available that provide additional analysis capabilities. This section also presents analysis of retrieved aerosol properties as compared to the specified ground truth that served

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as input to the simulations. Finally, section 5 discusses the next steps in the continuing MCARS development.

2 GEOS-5 aerosol model and data assimilation systems

2.1 System Description

Global aerosol, cloud, surface and atmospheric column fields from the GEOS-5 model and data assimilation system serve as the starting point for radiance simulations. The GEOS-5 system contains components for atmospheric circulation and composition (including aerosol and meteorological data assimilation), ocean circulation and biogeochemistry, and land surface processes. Components and individual parameterizations within components are coupled under the Earth System Modeling Framework (ESMF, Hill et al. 2004). This study is based on the near real-time (NRT) configuration of GEOS-5 where sea surface temperature and sea ice are specified from observations (Molod et al. 2012). The GOCART bulk aerosol scheme currently used in the GEOS-5 NRT aerosol forecasting system is used for the simulations reported in this paper. A version of the Goddard Chemistry, Aerosol, Radiation, and Transport model (GOCART, Colarco et al. 2010, Chin et al. 2002) is run online and radiatively coupled in GEOS-5. GOCART treats the sources, sinks, and chemistry of dust, sulfate, sea salt, and black and organic carbon aerosols. Total mass of sulfate, and hydrophobic and hydrophilic modes of carbonaceous aerosols are tracked. Dust and sea salt have an explicit particle size distribution with five non-interacting size bins for each constituent. Emission functions of both dust and sea salt depend on wind speed. Sulfate and carbonaceous species have contributions primarily from fossil fuel combustion, biomass burning, and biofuel consumption, with additional biogenic sources of organic carbon. Sulfate has additional chemical production from oxidation of SO_2 and dimethyl sulfide (DMS). We

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additionally include a database of volcanic SO_2 emissions and injection heights. For all aerosol species, optical properties are obtained primarily from the commonly used Optical Properties of Aerosols and Clouds (OPAC) data set (Hess et al. 1998). We have recently updated our dust optical properties data set to incorporate non-spherical dust properties based on the work of Meng et al. (2010), Colarco et al. (2014) and Buchard et al. (2014). The GOCART modules are run online within the GEOS-5 atmospheric general circulation model (AGCM); that is, the aerosols and other tracers interact radiatively and their transport is consistent with the underlying atmospheric dynamics and physical parameterizations (e.g., moist convection and turbulent mixing) of the model.

The GEOS-5 meteorological data assimilation is based on the Grid-point Statistical Interpolation (GSI) analysis scheme, jointly developed with National Oceanic and Atmospheric Administration National Center for Environmental Prediction (NOAA/NCEP) (Wu et al. 2002; Kleist et al. 2009). While the current GEOS-5 operational algorithm is based on a hybrid ensemble-variational scheme, the results reported here are based on the original 3D-Var implementation (Rienecker et al 2008). The current system uses the GEOS-5 Goddard Aerosol Assimilation System (GAAS, Buchard et al. 2015). GAAS analyzes the five primary GOCART aerosol species (15 total tracers) including black and organic carbon, dust, sea salt and sulfates. The analysis is produced at three-hour intervals, with assimilation of bias-corrected aerosol optical depth (AOD) from several ground- and satellite-based sensors including the Moderate Resolution Imaging Spectroradiometer (MODIS), Multi-angle Imaging Spectroradiometer (MISR) over bright surfaces, and the Aerosol Robotic Network (AERONET).

2.2 Fire Emissions

The fire emissions used in our simulations come from the Quick Fire Emission Dataset (QFED) Version 2.4 (Darmenov and da Silva, 2015). The QFED emissions are based on a top-down approach relating satellite retrieved Fire Radiative Power (FRP) at the top of the atmosphere to the amount of gases and particulate matter being emitted at the burning surface. The QFED emission factors are tuned as to promote agreement among modeled and observed AOD. Another unique feature of QFED is how it handles areas obstructed by clouds when estimating grid-box mean emission rates. A sequential, minimum-variance algorithm keeps track of the fractional obscured area of given grid box. Emissions under the obscured area are then obtained by means of damped persistency model. Details can be found in Darmenov and da Silva (2015).

2.3 Case study selection

The WMO's Working Group on Numerical Experimentation (WGNE) has organized an exercise to evaluate the impact of aerosols on Numerical Weather Prediction (NWP) (Freitas et al. 2015.) This exercise involves testing of regional and global models currently used for weather forecasting by operational centers worldwide. The authors of this exercise selected 3 strong or persistent events of aerosol pollution worldwide that could be fairly represented by current NWP models. These cases were specifically selected to facilitate evaluation of the aerosol impact on weather prediction. We chose one of the specified WGNE events: an extreme case of biomass burning smoke in Brazil as focus of this paper.

3 MODIS aerosol product

The MODIS "dark-target" (DT) aerosol product is described in detail in Levy, et al. (2013) and references therein. In this section we will give a brief overview of the DT algorithm as applied to MODIS observations.

The MODIS DT aerosol retrieval follows a lookup table (LUT) approach, meaning that satellite observations of TOA spectral reflectance are compared with pre-computed simulations of the TOA reflectance for aerosol scenes. A necessary constraint for the algorithm is that the surface is dark or otherwise well constrained in visible and shortwave-IR wavelengths. Since ocean and land optical properties are significantly different, the DT algorithm is in fact two separate algorithms, one over ocean and the other over land.

Each MODIS granule is a five-minute aggregation of pixels, nominally 1354 x 2330 (roughly1 km resolution at nadir). The standard algorithm works on boxes of 10x10 pixels, so that the final product is 134 x 203 pixels. If a 10x10 box is 100% ocean the ocean algorithm is followed, otherwise the land algorithm is attempted. Whether over ocean or land, these steps are followed.

1) Out of the 10x10 pixels, use a combination of the so-called Wisconsin cloud mask (MxD35_L2; Ackerman et al., 2006) and internal "aerosol" tests based on 3x3 pixel variability and 1.38μm cirrus reflectance threshold test to discard pixels that are definitely "cloudy".

2) Discard pixels that may be too bright for aerosol retrieval, and pixels that may be contaminated by ice/snow, sun glint, underwater sediments (ocean) or ephemeral water (land).

3) Collect the remaining pixels and discard a certain fraction (reducing potential contamination of clouds and cloud shadows).

4) Average the remaining pixels to create an array of TOA spectral reflectance that represents the 10 km box.

5) Perform algorithm to retrieve aerosol optical depth (AOD) and fine-mode aerosol weighting (FMW), based on finding which set of simulated spectral TOA reflectance best matches the observed TOA values.

6) Estimate quality-assurance confidence levels and other diagnostics related to the

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aerosol retrieval.

While all steps are performed for retrieval over either surface, it is the complexities of these individual steps that make aerosol retrieval difficult.

For the retrieval over ocean, the algorithm takes advantage that the ocean surface tends to be dark at wavelengths $\lambda \geq 0.55$ μm. This leads to robust separation of the aerosol signal and small uncertainties in retrieving AOD. Over land, although there is much more uncertainty as to the land surface optical properties, aerosol retrieval is still achievable. Over vegetated and dark-soiled surfaces, Kaufman et al. (1997) found that surface reflectance values for red (e.g. 0.65 μm) and blue (0.47 μm) wavelengths are correlated with the surface reflectance in a short-wave infrared (SWIR) band (e.g. 2.11 μm). Levy et al. (2007) found that additional spectral information could improve the relationship. Therefore, since AOD tends to be low in the SWIR, we can assume that the SWIR surface reflectance is approximately the observed TOA reflectance, so that the visible channel surface reflectance can be estimated. As a result, the over-land aerosol algorithm uses three bands for retrieval (0.47, 0.65 and 2.1μm), but uses additional bands (0.55, 0.86 and 1.24 μm) to provide better constraints on the surface properties.

The aerosol LUT is calculated for black surfaces and sea-level pressure. There are three fine particle model types and one coarse particle model type of aerosols based on climatology of AERONET inversion data (Dubovik et al, 2002). Each model type is multi-lognormal and is represented by size distribution, particle shape and complex refractive indices. The three fine-dominated models are all spherical in shape and differentiated primarily by single scattering albedo (SSA) in mid-visible wavelengths. These include a weakly absorbing type (SSA~0.95) representing urban/industrial aerosol, a strongly absorbing type (SSA~0.85) representing near-source biomass burning smoke, and a moderately absorbing type (SSA~0.90) representing boreal smokes and everything else that is not either of the other two

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types. The single coarse-dominated aerosol type is non-spherical and represents dust-like type. For each aerosol type, the LUT includes TOA reflectance calculations for a number of discrete aerosol loadings (function of AOD at 0.55 ranging between 0.0 and 5.0) at the three wavelengths (0.47, 0.65 and 2.1µm), and a number of possible angle combinations (sensor and solar geometry).

Even with the constraints on surface reflectance, the aerosol retrieval does not have enough information to select between different aerosol types. Therefore, the fine-model and coarse-model aerosol types are prescribed as a function of season and location. The retrieval algorithm picks the relative weighting (FMW) of fine-model (prescribed) and coarse model (prescribed as dust) and loading (AOD at 0.55 µm) that, coupled with the surface reflectance constraints, best matches the TOA spectral reflectance in the blue, red and SWIR wavelengths. The difference between TOA and simulated reflectance is the fitting error.

With Levy et al., (2013) and previous studies, the primary validation of the MODIS product is by detailed co-location with ground-based sun photometer data, especially the Aerosol Robotic Network (AERONET; Holben et al., 1998). In this way, Levy et al., (2013) has defined the expected error (EE) envelope for the 0.55 µm AOD as ±(0.05 + 15%;). While spectral surface reflectance is also retrieved, it does not tend to compare well with values obtained from the sun photometers.

Note that the EE is defined upon mutually retrieved data. This means that satellite and sun photometer both observe enough clear-sky to retrieve AOD. There are many cases where either MODIS or AERONET were not able to make a retrieval or observation. Such cases where only one value is available are not included in the co-location dataset. For example, consider scenes of popcorn-type cumulus clouds. If MODIS retrieval is unsuccessful due to having too many cloudy pixels in the 10x10 sample box, but AERONET managed to observe between the clouds, we would never know about the cloud contamination. On the other hand,

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MODIS may be completely successful at removing the cloudy pixels, but AERONET does not retrieve because of perceived clouds in its scene. We would never be able to discern that kind of contamination either.

Also, while AERONET is well distributed about the globe, there are many situations for which MODIS retrieves aerosol, but there is no AERONET data available to compare with. Thus, there is no way to determine whether the MODIS aerosol retrieval has made reasonable choices, either for pixel selection, for cloud screening, or for aerosol model type and surface reflectance assumptions.

This motivates our use of the MCARS. Having full knowledge of underlying atmospheric, cloud, aerosol and surface parameters MCARS allows us to see deeper than AERONET would over a wide spatial area.

4 MCARS simulations

4.1 The MCARS software

We produced the simulation input data in accordance with the methods outlined in (Wind et al, 2013). The GEOS-5 model output is split into 1-km subcolumns using the independent column approximation (ICA) method as described in Wind et al. (2013). In particular, relative humidity field used to compute aerosol hygroscopic effects is sub-sampled using a probability distribution function (PDF) representation of total water. Model parameters such as profiles of temperature, pressure, ozone and water vapor together with layer information about clouds (and now aerosols) are combined with solar and view geometry of the MODIS instrument. Surface information is also a combination of GEOS-5 information of surface temperature, snow and sea ice cover and MODIS-derived spectral surface albedo (Moody et al. 2007, 2008). All these parameters are transferred to the DISORT-5 radiative transfer code and reflectances and radiances in 24 MODIS channels are produced. They are output into a standard MODIS L1B file that corresponds to the source MODIS geolocation file we used to sample the model output with. All metadata is preserved in this process and so the MCARS output is indistinguishable from a real MODIS granule except in how it may appear to the user's eye. These synthetic reflectances and radiances are completely transparent to any operational or research-level retrieval algorithm code and can be used for any purpose that real sensor data can.

4.2 Granule selection

In order to perform tests of the MCARS aerosol module we have selected Aqua MODIS granules from time period corresponding to WGNE selection for biomass burning in Brazil. In this paper we specifically present results from simulations based on two granules of smoke in Brazil 2012 day 252 17:30 UTC and day 254 17:20 UTC subsequently referred as "Brazil 1" and "Brazil 2".

5 Analysis

For each granule, we ran the simulations in several modes with varied run option settings. For example, the cloud-only mode corresponds to a clean atmosphere with no aerosols; this mode was the only one considered in Wind et al. (2013). In the current paper we consider additional options afforded by the implementation of the aerosol effect. The cloud-free option runs atmosphere and aerosols without any clouds. When clouds are turned off, we do not alter the humidity profiles to dry the atmosphere out; because of the high relative humidity conditions where clouds are present, aerosol hygroscopic effects are pronounced there as well. The full simulation option includes atmosphere (temperature, humidity and ozone profiles), all clouds and all aerosols. There is also an additional option where the user can remove both clouds and aerosols and be left with just the atmosphere itself. While this no-cloud/no-aerosol mode could be useful for studies of atmospheric correction methods, we do

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not exercise it here, as our primary goal here is to investigate the performance of the MODIS aerosol algorithms.

The cloud-free mode of operation is convenient when complex cloud and aerosol scenes are being investigated and one wishes to quantify or remove possible impacts of cloud contamination on the retrieval. Figure 1 shows RGB images constructed from simulated MODIS L1B for the different modes of execution for the "Brazil 1" case. MODIS aerosol retrievals were produced for radiance simulations including atmosphere, cloud and aerosols (Figure 1c) and for radiance simulations excluding clouds (Figure 1d).

These Brazil cases came from source MODIS Aqua granules and had been processed using the MODIS Aqua aerosol properties retrieval algorithm. Therefore in this section we will use MYD04 designation for the MODIS aerosol properties retrieval result. There are some slight differences between the MODIS Terra (MOD04) and MODIS Aqua (MYD04) algorithms due to calibration differences between the two instruments (Levy et al, 2013).

The scatter diagrams in Figure 2 compare AOD retrieved using the MYD04 algorithm to the specified GEOS-5 AOD, which is considered the ground truth in this case. Such comparisons are to be contrasted to similar comparisons between MODIS aerosol retrievals and co-located AERONET AOD measurements (Correia and Pires 2006, Levy, et al. 2007b, Remer et al. 2005). Unlike comparisons of actual MODIS data with AERONET, the match ups in Figure 2 did not require any temporal averaging or aggregation because for every MYD04 retrieval there is a directly corresponding input data point with all aerosol, cloud and atmospheric properties readily available. The overall shape of resulting scatter plots turned out to be quite similar to existing MYD04 – AERONET comparisons for this region such as those that appear in Correia and Pires (2006) and Figure 3. Figure 3 shows a comparison for AERONET observations for months of July and August of all available Aqua MODIS collocated observations from year 2002 through 2015. The chosen AERONET sites:

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Campo_Grande_SONDA, Sao_Paulo and CUIABA-MIRANDA fall in the general area of the two Brazil cases selected for study. They of course represent a tiny sample of the geographical area covered by the MCARS data, just three points out of 2.7 million collocated samples that MCARS provides, but they display a similar shape of the relationship between ground truth and MYD04 retrieval.

MCARS is a fully configurable system where source input for all synthetic radiances can be controlled at all times, so that any resulting retrieval can be examined in great detail. For these smoke cases we used these capabilities to investigate further the specific reasons why the MYD04 retrievals tend to underestimate AOD for smoke aerosol.

The first test we made was to examine the performance of MYD04 cloud mask, which is an aerosol specific product (Remer et al, 2005), different from the operational MODIS cloud mask product (Ackerman et al, 2006). The main purpose of this analysis was to ascertain whether cloud contamination could account for some of the discrepancies. Individual panels in Figure 2 show the results of retrievals run with and without the cloud layers. Panels a) and b) show result for “Brazil 1” and panels c) and d) are for “Brazil 2”. “Brazil 1” case does not show any significant cloud contamination. The MYD04 cloud mask does a very good job of avoiding cloud. “Brazil 2” does show some very minor cloud contamination as evident by a small cluster of high MYD04 AOD and low GEOS-5 AOD that disappears when clouds are removed from simulation. However the overall shape of scatter plot when clouds are removed remains unchanged.

The aerosol models used in the MYD04 retrievals make assumptions about the smoke aerosol optical properties, which may not match the aerosol optical assumptions in GEOS-5 (Levy et al, 2007). In cases of complex aerosol mixtures or if the model selected by the MYD04 algorithm does not correspond to the aerosols provided by GEOS-5, large retrieval errors should result. Figure 4 shows the species mixture for “Brazil 1” (a) and “Brazil 2” (b)

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cases. They are both dominated by carbon, organic carbon from smoke in particular, with very little, if any contribution from other species. Therefore these particular cases can be treated as having a single aerosol type present without significant error. MYD04 retrieval output indicates that either moderately or strongly absorbing smoke had been selected, which is very appropriate for the selected granules. Thus any discrepancy in selection of aerosol model does not explain the scatter plot shape.

Another candidate source of retrieval error is any difference between the phase functions assumed by MYD04 and GEOS-5. We ran the initial simulations simply using the Henyey-Greenstein (HG) phase function approximation and then repeated the same simulation using the phase functions provided by the OPAC database described in section 2. Figure 5 shows the result for "Brazil 1" and "Brazil 2" cases using the cloud-free run with HG phase function versus OPAC phase function. For the smoke aerosol cases studied, the specific phase function shape does not appear to have a significant impact on the differences seen between MYD04 and GEOS-5.

An additional potential source of error for aerosol retrievals over land is the surface albedo and its variation over a 10x10 km area. We performed a simulation where we selected a single surface albedo profile from a successful MYD04 retrieval and fixed the surface albedo to that particular surface albedo profile for the entire granule. The test albedo profile used is listed in Table 1. The profile corresponds to a very dark vegetated surface, the ideal conditions for the MYD04 land algorithm. Figure 6 shows the effect of using a constant surface albedo for "Brazil 1" and "Brazil 2" cases. Whereas use of constant surface albedo reduces the scatterplot spread and so allows us to potentially quantify the effect of surface inhomogeneity on MYD04 land retrievals, it does not change the overall shape of scatter plot.

With all the factors of model selection, surface parameters and cloud contamination taken into account, we now turn our attention to the aerosol scattering properties, the spectral single

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scattering albedo (SSA) in particular. Figures 7 and 8 show the spectral profile of aerosol SSA for "Brazil 1" and "Brazil 2" cases respectively for the first seven MODIS channels. The single scattering albedo remains quite high until we reach the 1.2µm channel, MODIS band 5, and beyond. Then it drops precipitously. AERONET is only able to provide direct measurements up to 1.02µm (Holben et al, 1998). The rapid change in single scattering albedo for smoke aerosol modeled in GEOS-5 is related to aerosol humidification effects, both dilution effects and hygroscopic growth (Colarco et al. 2010, 2013). The net effect is that when humidity decreases, so does the single scattering albedo. Figure 9 shows a plot of OPAC single scattering albedo for a variety of column relative humidity values as a function of wavelength. (Colarco, et al 2013) The operational MODIS aerosol code assumes a constant 80% relative humidity when the lookup tables are generated (Levy et al, 2007). It is a good assumption as long as one does not attempt to use channels with wavelengths that are longer than 0.8µm. The MYD04 algorithm however does use the 2.1µm MODIS channel during retrieval, a channel that is sensitive to humidity. MCARS is particularly well suited to test for humidity impact on the retrieval accuracy. We made another experiment with fixed surface albedo, OPAC aerosol phase function shape but we used the constant single scattering albedo values from the MODIS aerosol algorithm in the reflectance calculation that serves as input to the retrieval algorithm. The result is shown in figure 10. When humidification effects are not taken in consideration in the SSA calculation, MYD04 retrieval result lines up with "ground truth" GEOS-5 source data. The underestimate of aerosol optical depth disappears, with "Brazil 2" showing the most dramatic improvement. It appears that if MYD04 were to take into account humidification effects and implement a correction for single scattering albedo value as a function of column relative humidity, the result of comparison between MODIS and AERONET could be significantly improved for biomass burning cases in Brazil and other locations with similar synoptic conditions.

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MODIS aerosol product performs a simultaneous retrieval of land surface reflectance and aerosol optical depth. After looking at behavior of aerosol optical depth and making a recommendation for a possible improvement in retrieval algorithm, we examined the retrieval of land surface reflectance. MODIS aerosol product provides retrieved land surface reflectance in the 0.47, 0.65 and 2.1μm channels. We looked at the land surface reflectance for the simulation of figure 10 panels b) and d) that now matched the source aerosol optical depth reasonably well. The simulation was run under constant surface albedo conditions and we would have expected to see a result, with some degree of uncertainty of course, that would match the given constant surface albedo. However the retrieved land surface reflectance appeared to be a near-linear function of aerosol optical depth. One possible explanation for this behavior may involve the assumed fraction of coarse-mode aerosol in the aerosol model mixture. To examine this hypothesis we performed a MYD04 retrieval using an aerosol model setting so that MYD04 retrieval only used fine mode particles. The retrieval results, depicted in figure 11 confirm that the near co-linearity of surface reflectance and AOD was indeed directly related to fraction of coarse mode particles, such as dust, in the assumed aerosol mixture. Of course there is no way to know exactly what fraction of coarse mode particles may be present in the mixture as the MODIS dark target algorithm does not have enough information content to constraint the fine/coarse mode fraction over land (Levy et al, 2007). However, it can be noted that if such co-linearity is seen during a specific local aerosol study maybe during a field campaign, it may be suggested that the coarse mode fraction assumed operationally for that particular region may be too high. An analysis of MODIS operational retrievals to identify locations and times where this co-linearity exists may be useful to identify regions where the assumed coarse/fine mode fraction might need to be adjusted. Figure 11 illustrates the impact of coarse-mode fraction selection on “Brazil 1” and “Brazil 2” cases. The fine-to-coarse mode ratio does not appear to have an impact on the shape of

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MYD04 vs. "ground truth" comparison.

6 Conclusions and future directions

This paper is a continuation of work started in Wind et al, (2013). The multi-sensor cloud retrieval simulator code (MCRS) had been extended to add aerosol effects to radiance simulations. The current implementation of the MCARS code generates synthetic radiances by sending GEOS-5 model fields and MODIS sensor geometry and location information to DISORT-5 radiative transfer core. The radiance and reflectance data is output in a standard MODIS Level 1B format that can be transparently ingested by any retrieval or analysis code that reads data from the MODIS instrument.

After the aerosol properties module had been added to the MCARS code we used the simulator to perform detailed analysis of performance of the operational MODIS dark target aerosol properties retrieval product for the Aqua MODIS instrument (MYD04). We found the cause of known low bias in MYD04 retrieved aerosol optical depth for smoke when compared to in-situ measurements. We suggest that the MYD04 retrieval should take into account column relative humidity when performing retrievals in regions that are defined to be dominated by smoke aerosols. The mismatch between the aerosol single scattering albedo assumed by MYD04 and the "ground truth" single scattering albedo is the cause of the low bias.

This study is a good example of capabilities of the MCARS code. We are planning many more studies of retrieval algorithm performance. On the other hand, the MCARS results give a relationship between aerosol single scattering albedo, bias in retrieved aerosol optical depth and column relative humidity.

One of our future directions is to examine further this relationship and possibly establish a solid parameterization that could be used by the modeling community to reduce biases in assimilated observations that might display a similar low bias when compared to in-situ

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measurements.

There are many other potential applications of the MCARS code, including extending the simulator to sensors other than MODIS.

7 Code and Data Availability

The MCARS code and any datasets produced, including all data shown (GEOS-5 input in netCDF4 and all MODIS output in HDF4 file format) and discussed in this paper, are available to users free of charge by contacting the authors and becoming a registered user of this software package so that any updates to code or datasets can be issued directly. There may be additional, wider distribution means in the future as needed. We have not deemed it practical up to this time to release the MCARS source code into general-purpose source repositories. The data files are quite large with source input data being on the order of 20 Gb for each MODIS-like granule created. The GEOS-5 model source code is publicly available and we may release the MCARS code under the same NASA Open Source Agreement and the same repository in the coming year.

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Table 1: Constant surface albedo setting used in smoke AOD retrieval investigation

MODIS channel	Surface Albedo
1	0.027
2	0.288
3	0.017
4	0.037
5	0.252
6	0.146
7	0.054
8	0.014
9	0.022
17	0.283
18	0.280
19	0.280
20	0.038
22	0.038
26	0.216

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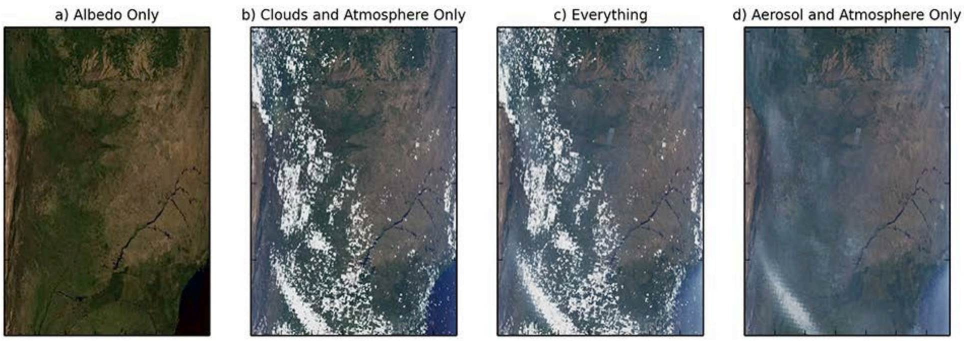

Figure 1. Example of various execution modes of the MCARS code using the "Brazil 1" case 2012 day 252 17:30UTC. Panel a) shows the atmosphere-free image, basically the surface albedo. Panel b) shows the clouds-only simulation with no aerosols. Panel c) has both clouds and aerosols and panel d) shows the cloud-free mode, where cloud layers have been removed from the scene

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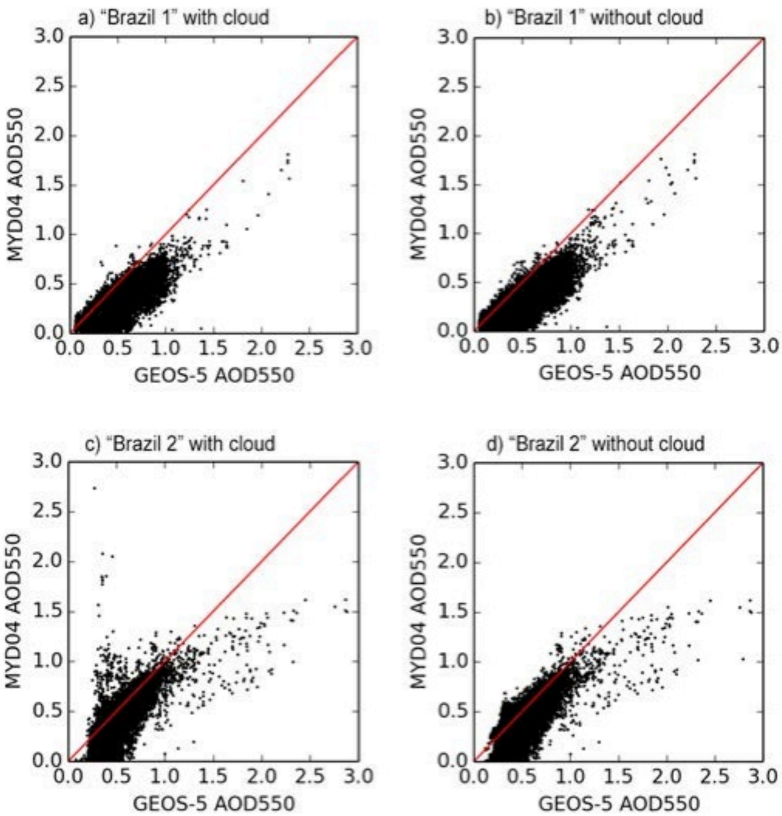

Figure 2. MYD04 retrieval vs ground "truth" of GEOS-5 aerosol optical depth. Panel a) shows the scatterplot for retrieval from simulation in figure 1c and panel b) shows retrieval from simulation in figure 1d for "Brazil 1" case. Panels c) and d) show same information for "Brazil 2" case.

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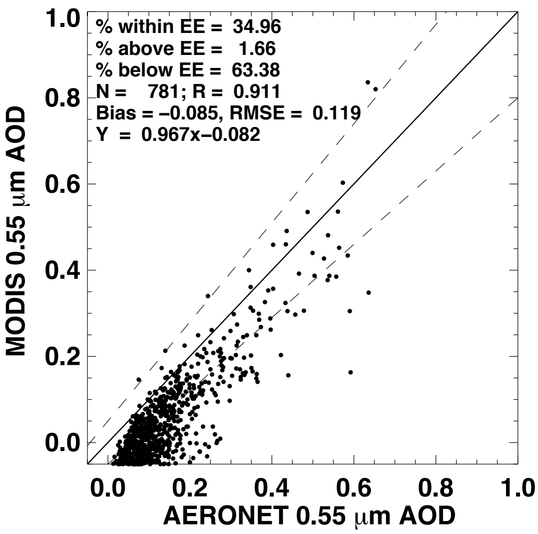

Figure 3. Comparison of actual AERONET measurements and operational Aqua MODIS Collection 6 aerosol product for Brazil sites Campo_Grande_SONDA, Sao_Paulo and CUIABA-MIRANDA in the general area of MCARS granules.

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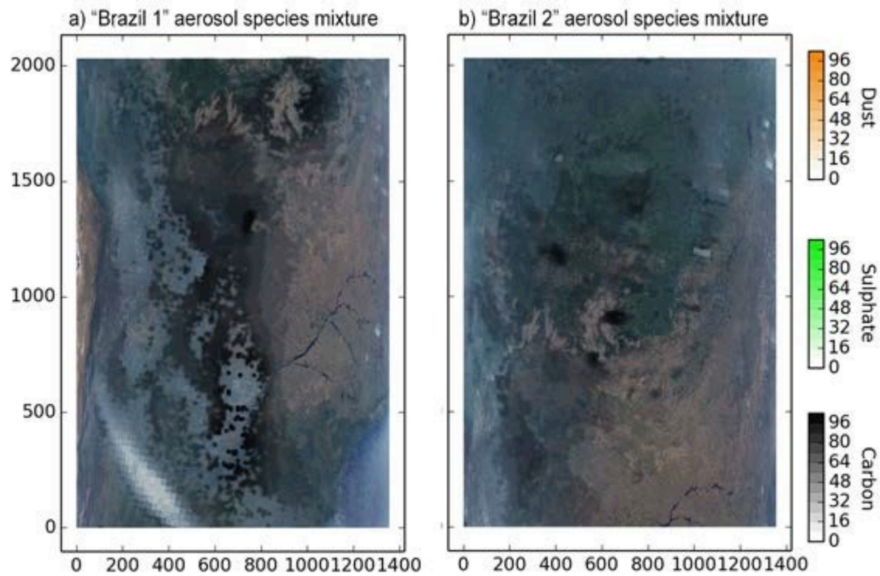

Figure 4. GEOS-5 aerosol species mixture for attempted MYD04 retrievals in figure 2. Panel a) shows the "Brazil 1" case (2012 day 252) and panel b) shows the "Brazil 2" case (2012 day 254). Both are dominated by carbon (smoke) aerosol.

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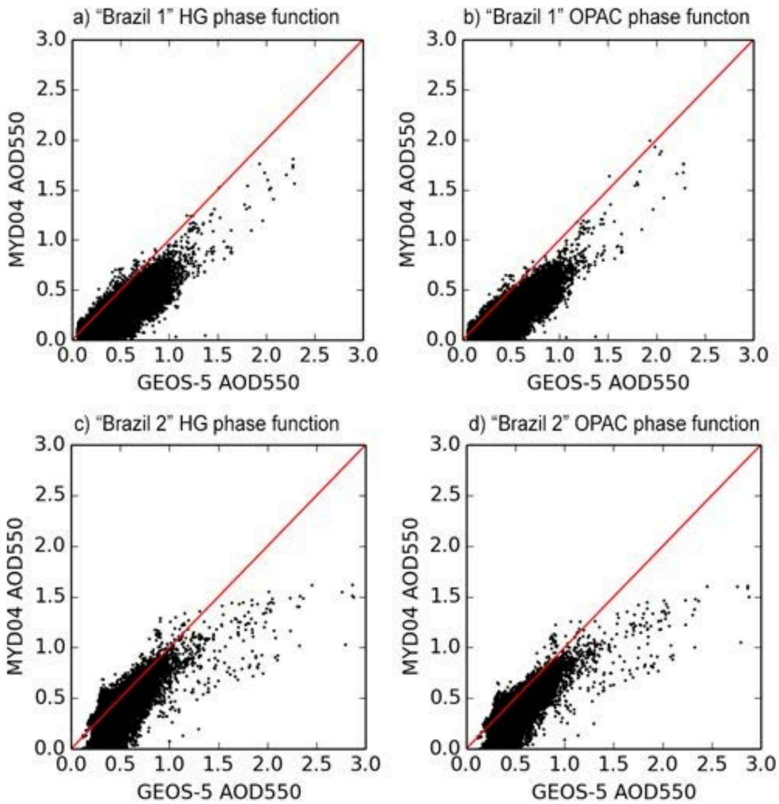

Figure 5. Effect of aerosol phase function shape on Brazil smoke cases. Panels a) and c) show the runs with HG phase function. Panels b) and d) show use of the OPAC composite phase function.

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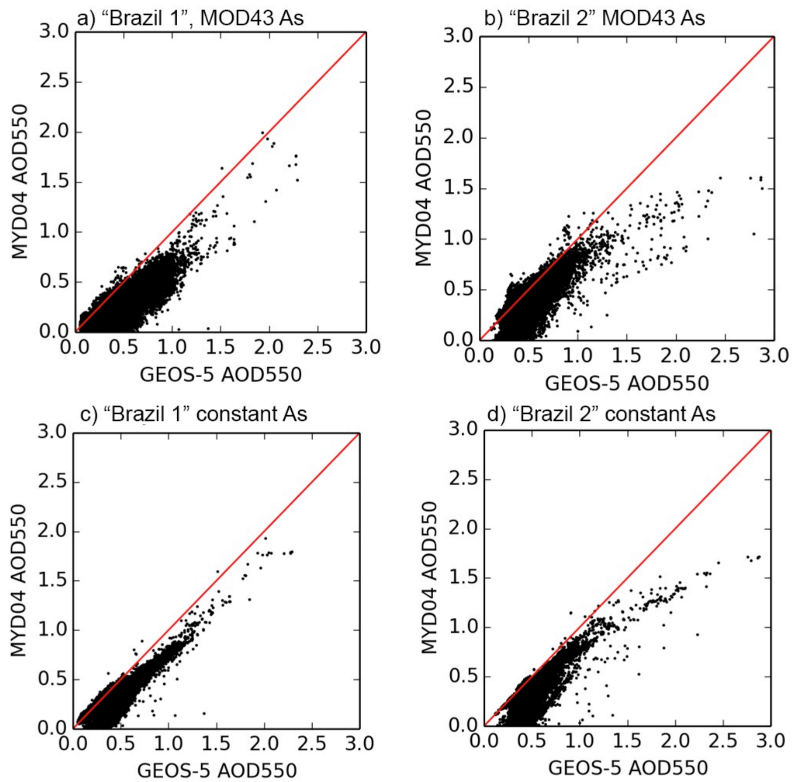

Figure 6. Surface albedo effect on Brazil smoke cases. Panels a) and c) show the runs with MOD43-derived surface albedo. Panels b) and d) show the effect of selection of a constant dark land surface albedo.

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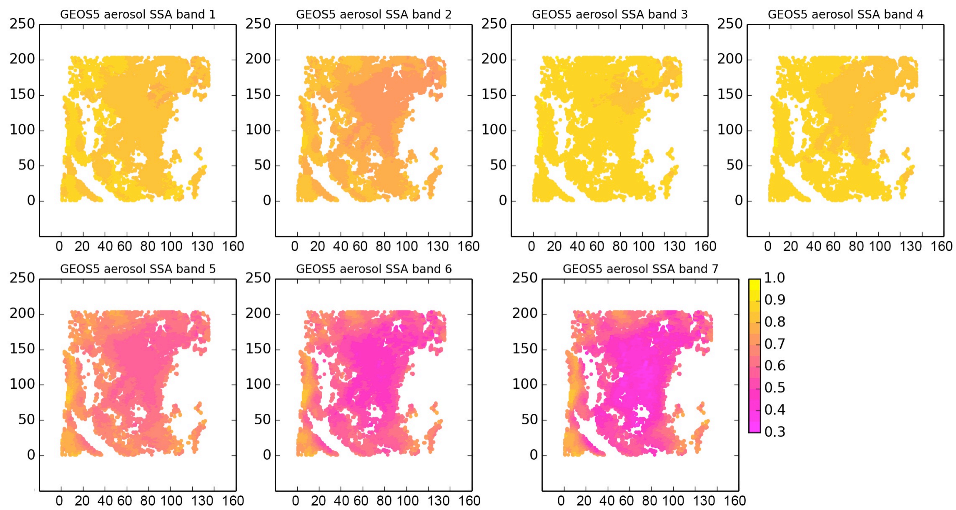

Figure 7. Aerosol single scattering albedo for “Brazil 1” case for MODIS channels 1-7.

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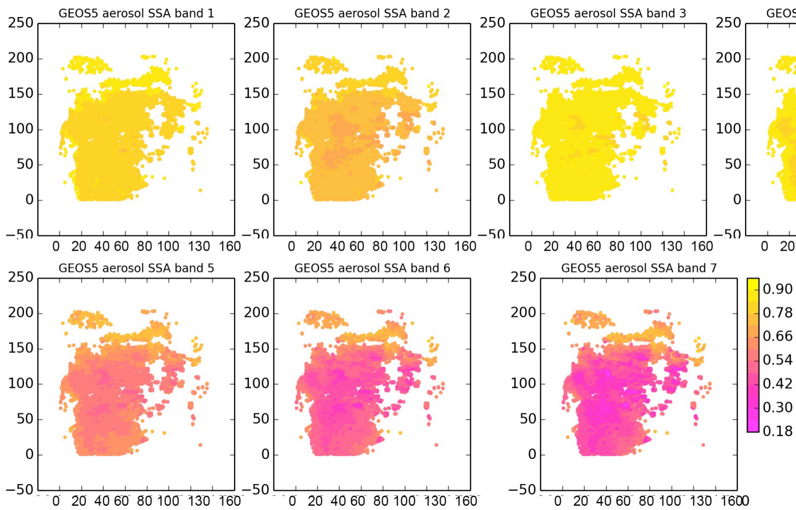
1 

2 Figure 8. Aerosol single scattering albedo for “Brazil 2” case for MODIS channels 1-7.

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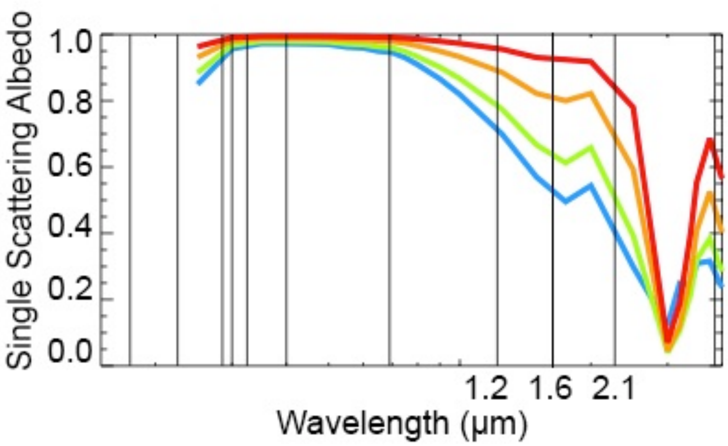

Figure 9. OPAC single scattering albedo as a function of humidity (color) and wavelength. The various relative humidity levels are in order (red, orange, green and blue) for 95, 80, 30 and 0% column relative humidity.

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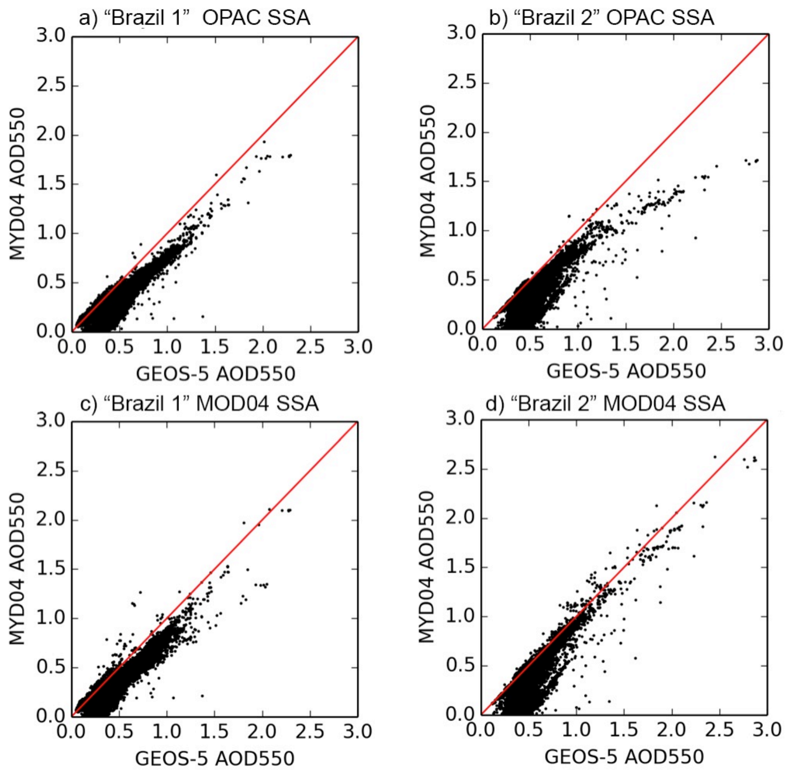

Figure 10. Impact of humidity on MOD04 retrieval illustrated via single scattering albedo selection. Panels a) and c) show the “Brazil 1” case before and after the SSA adjustment. Panels b) and d) show the same for “Brazil 2”.

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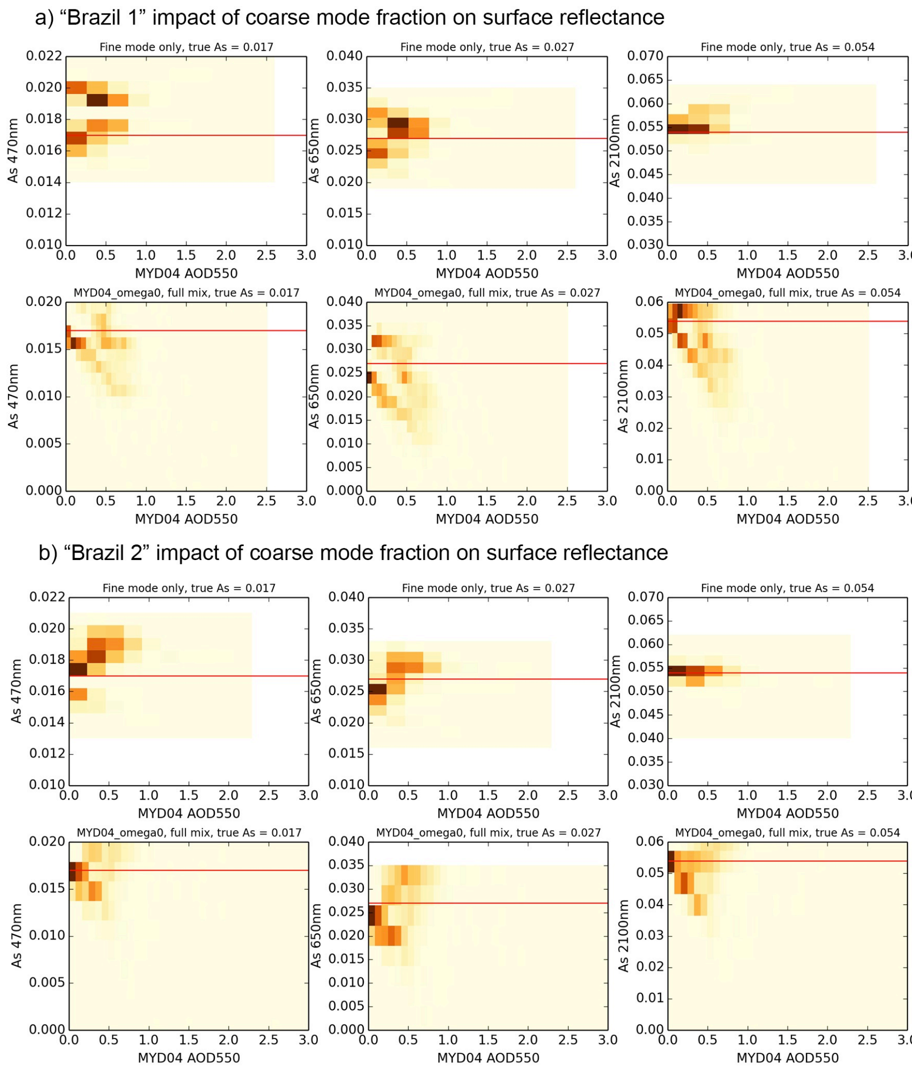

Figure 11. Impact of coarse mode fraction on MOD04 retrieved surface reflectance. Set a) shows the "Brazil 1" case and set b) shows "Brazil 2".