

# NOAA NESDIS CENTER for SATELLITE APPLICATIONS and RESEARCH

# GOES-R Advanced Baseline Imager (ABI) Algorithm Theoretical Basis Document

# For

# Suspended Matter/Aerosol Optical Depth and Aerosol Size Parameter

NOAA/NESDIS/STAR

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AAA	Aerosol, Air Quality and Air chemistry
ABI	Advanced Baseline Imager
AERONET	AErosol RObotic NETwork
AIT	Algorithm Integration Team
AOD	Aerosol Optical Depth
ASP	Aerosol Size Parameter
ASTER	Advanced Space Thermal Emission and Reflection Radiometer
ATBD	Algorithm Theoretical Basis Document
ATIP	Algorithm and Test Implementation Plan
AWG	Algorithms Working Group
BRDF	<b>Bi-directional Reflectance Distribution Function</b>
CONUS	Continental US
FMW	Fine Mode Weight
F&PS	Functional and Performance Specification document
GFS	Global Forecast System
GOES	Geostationary Operational Environmental Satellite
IMS	Interactive Multisensor Snow and Ice Mapping System
JPSS	Joint Polar Satellite System
LUT	Lookup Table
MODIS	Moderate Resolution Imaging Spectroradiometer
MRD	Mission Requirements Document
NASA	National Aeronautics and Space Administration
NCEP	National Centers for Environmental Prediction
NDVI	Normalized Difference Vegetation Index
NESDIS	National Environmental Satellite, Data, and Information Service
NIR	Near Infrared
NOAA	National Oceanic and Atmospheric Administration
NPOESS	National Polar-orbiting Operational Environmental Satellite System
NWS	National Weather Service
PDF	Probability Distribution Function
	Probability Distribution Function Particulate Mass of particles smaller than 2.5 µm in median
PM2.5	diameter
PORD	Performance and Operation Requirements Document
RMS	Root Mean Square
RTM	Radiative Transfer Model
SWIR	Shortwave Infrared
SEBN	Surface Energy Balance Network
SEVIRI	Spinning Enhanced Visible and Infra-red Imager
TOA	Top of Atmosphere
TPW	Total Precipitable Water
UMBC	University of Maryland Baltimore County
VIIRS	Visible/Infrared Imager/Radiometer Suite
VIIKS	Visible/Inflated Inflager/Radiometer Suite
v 15	v isibile

## ABSTRACT

Atmospheric aerosols (liquid or solid particles suspended in the air) affect the radiative energy budget, the hydrological cycle, atmospheric circulation, land surface processes, and climate. They also play a role in air quality and have an impact on human health. Largescale continuous characterization of atmospheric aerosols relies upon satellite remote sensing.

This document describes the algorithm designed for retrieving aerosol properties from multispectral reflectances observed by the Advanced Baseline Imager (ABI) onboard the geostationary satellite GOES-R. The ABI aerosol algorithm retrieves the aerosol optical depth, suspended matter and aerosol size parameter at 2-km spatial and 5- and 15- minute temporal resolutions over the CONUS and full-disk domains, respectively, under daytime clear-sky conditions. Separate algorithms have been developed for the retrieval over land and over ocean due to the distinct surface properties and aerosol types. To aid rapid retrieval of aerosol properties, look-up tables of spectral atmospheric (aerosols plus molecules) optical functions (reflectance, transmittances and spherical albedo) are precalculated for a wide range of geometries and standard aerosol models at standard surface pressure. Over land, surface reflectance in the visible spectrum is obtained from the shortwave infrared reflectance based on pre-determined spectral relationships. Over ocean, the surface reflectance is modeled as the sum of underwater, whitecap, and sun glint direct reflection. Top of the atmosphere (TOA) reflectance is calculated from coupling the surface and atmospheric reflections, which is then compared with observations to determine the optimal solution for aerosol optical depth and aerosol type. The suspended matter is determined from the retrieved aerosol optical depth applying the mass extinction coefficient indicated by the aerosol model retrieved simultaneously with the optical depth. Aerosol size parameter (Ångström Exponent) is calculated from retrieved spectral aerosol optical depths. Pre-launch validation of the ABI algorithm was performed with proxy data from MODIS. The retrieved aerosol optical depth and Ångström exponent were compared with ground measurements from AERONET. The comparisons indicated compliance with requirements for aerosol optical depth. Accuracy of Ångström exponent also meets the requirement, but the precision does not.

## **1 INTRODUCTION**

Aerosols are liquid or solid particles suspended in the atmosphere. Aerosols modify the energy budget of the earth-atmosphere system in several ways. They directly scatter and absorb solar and thermal infrared radiation [e.g., Bohren and Huffman, 1983; Coakley et al., 1983; Charlson et al., 1992]; modify cloud amount, life time, and microphysical and radiative properties and therefore indirectly change the Earth-leaving radiation [e.g., Twomey, 1977; Albretch, 1989; Rosenfeld and Lensky, 1998]. Absorption of radiant energy by aerosols leads to heating of the troposphere and cooling of the surface, which can change the relative humidity and atmospheric stability thereby influencing cloud formation and precipitation [Hansen et al., 1997; Koren et al., 2004; Ackerman et al., 2000]. Consequently, aerosols can influence land surface processes [Yu, et al., 2002], the global surface temperature [Coakley et al., 1983; Charlson et al., 1992; Ramanathan et al., 2001], climate and the hydrological cycle [Ramanathan et al., 2001], and ecosystems [Chameides et al., 1999]. As complex mixtures of particles and particle aggregates of varying chemical composition, aerosols also affect regional air quality and human health [Pope et al., 2002]. Epidemiological studies have linked exposure to PM2.5 (particulate mass in units of  $\mu g/m^3$  of particles smaller than 2.5  $\mu m$  in median diameter) to a range of adverse health effects such as strokes, heart disease, respiratory ailments, and premature death [e.g. http://www.epa.gov/region4/sesd/pm25/p2.html].

Aerosols have high spatial and temporal variability due to the heterogeneous distribution of sources, short lifetime, and episodic feature of emission events. Therefore, continuous global and regional characterization can only be realized through satellite remote-sensing. Real time monitoring of aerosol optical depth from the Geostationary Operational Environmental Satellite (GOES) data are routinely conducted at the National Oceanic and Atmospheric Administration (NOAA). The algorithm prior to GOES-R uses only a single channel to retrieve aerosol optical depth (AOD). The need for using a single fixed aerosol model in this algorithm and the one-wavelength AOD do not allow estimation of size parameter. Moreover, relatively large uncertainty in the estimated surface reflectance leads to inaccurate AOD for certain times and regions. The Advanced Baseline Imager (ABI) flown on the GOES-R series of NOAA geostationary meteorological satellites measures radiances in multiple wavelengths from the UV through the IR at high spatial resolution [Schmit et al., 2005]. In contrast to the one channel used by the current GOES, GOES-R ABI has five channels between 0.47 and 2.25 µm that can potentially be used for retrieving aerosol properties over land and ocean. Similar multi-channel instruments (Moderate Resolution Imaging Spectroradiometer, MODIS, and Visible/Infrared Imager/Radiometer Suite, VIIRS) have already been flown on various spacecraft, and algorithms for retrieving aerosol from the measurements of these instruments (e.g., Kaufman et al., 1997; Remer et al., 2006; Levy et al., 2007; Vermote et al., 2006; Jackson et al., 2013; Liu et al., 2013) are already available and have been tested. The ABI aerosol algorithm described in this ATBD borrows heavily from these heritage algorithms.

#### 1.1 Purpose of This Document

The Algorithm Theoretical Basis Document (ATBD) describes the theory and necessary assumptions for deriving aerosol properties from ABI aboard GOES-R. Details of the algorithm, the products, and their uncertainties (as estimated from proxy and actual ABI data) are also discussed.

## **1.2 Who Should Use This Document**

The intended users of this document are those interested in understanding the physical basis of the algorithm and use the outputs of this algorithm in applications requiring aerosol data. This document also provides information useful to anyone maintaining or modifying the original algorithm.

### **1.3 Inside Each Section**

Specifically, this document is broken down into the following main sections:

- **Observing System Overview**: Provides the objectives of the algorithm, relevant characteristics of the instruments, and provides a brief description of the aerosol products generated by this algorithm.
- Algorithm Description: Provides detailed description of the physical and mathematical basis of the algorithm, the look-up tables, and inputs and outputs.
- Test Data Sets and Output: Describe the test data sets and processes to characterize the performance of the algorithm. This includes the method used for simulating proxy ABI data, algorithm output from the proxy ABI data, precision and accuracy estimates based on ground AERONET measurements, and error budget analysis.
- **Practical Considerations**: Provides an overview of the issues involving numerical computation, programming and procedures, quality assessment and diagnostics, and exception handling.
- Assumptions and Limitations: Provides an overview of the current limitations of the approach and gives the plan for overcoming these limitations with further algorithm development.

### **1.4 Related Documents**

GOES-R Mission Requirements Document (MRD) GOES-R Functional and Performance Specification Document (F&PS) GOES-R ABI Performance and Operation Requirements Document (PORD) GOSE-R ABI Suspended Matter/Optical Depth and Aerosol Size Parameter Algorithm and Test Implementation Plan (ATIP) Document GOSE-R ABI Suspended Matter/Optical Depth and Aerosol Size Parameter Product Validation Plan Document Product Definition and Users' Guide (PUG), Volume 5: Level 2+ Products, Revision E, 02 March 2017

### 1.5 Revision History

This is Version 4.3 (Jan 31, 2023) of the "GOES-R Advanced Baseline Imager (ABI) Algorithm Theoretical Basis Document for Suspended Matter/Aerosol Optical Depth and Aerosol Size Parameter" document. It describes the updated land surface reflectance relationships implemented in the GOES-R Algorithm Working Group (AWG) Version-6.3 algorithm, which improves representation of the diurnal cycle of GOES-16 AOD. A history of algorithm updates is listed in Table C-1. The Aerosol Particle Size Parameter (Ångström exponents at two pairs of wavelengths) over water has been included in the product since Sep 04, 2020.

Version 4.2 (Feb 14, 2018) and Version 4.1 (Jan 31, 2018) describe updates implemented in the AWG Version-6.1 algorithm package to reach product provisional maturity. It updates the land surface relationship based on ABI observations matched up with AREONET ground measurements. It is noted that the previous Version 6 algorithm expects ABI channel reflectances at their original resolution, but the Version 6.1 algorithm uses the ABI channel reflectances at 2 km resolution to facilitate faster implementation of the updates in the baseline AOD algorithm in the Ground System (GS).

Version 4.0 (Sep 30, 2016) describes updates implemented in Version-6 delivery of the algorithm package. Algorithms prior to Version 6 delivery assumed the ABI channel data were averaged to the required product resolution (2 km) before inputting to the algorithm. In contrast, the Version 6 algorithm expects ABI channel reflectances at their original resolution. The Version 6 algorithm also implements internal checks to screen out contaminated pixels and to identify low quality retrievals. It also updates the look-up-tables and channel related coefficients based on the most recent spectral response functions of the ABI channels.

The previous, Version 3.0 (June 30, 2012), ATBD was an update to Version 2.0 and followed the comments from the AER on Version 2.0 ATBD and reference codes.

Version 2.0 (Sep 25, 2010) evaluated the ABI aerosol algorithm to meet the 100% requirements and followed the comments on Version 1.0 from the ADEB and IV&V reviewers. It was written by members of the Aerosol Team, I. Laszlo, M. Zhou, H. Liu, and P. Ciren, of the GOES-R Algorithm Working Group (AWG) Aerosol, Air Quality and Air Chemistry (AAA) Application Team at NOAA/NESDIS/STAR.

Version 1.0 of this document was written for the 80% maturity delivery. That revision evaluated the algorithm to meet the 80% requirements and addressed the comments on the draft version (Version 0.0) from the project office. Version 0.0 was delivered on September

30, 2008 to accompany the delivery of version 1 of the algorithm to the GOES-R AWG Algorithm Integration Team (AIT).

## **2 OBSERVING SYSTEM OVERVIEW**

#### 2.1 Products Generated

The algorithm is designed to retrieve the aerosol optical depth (AOD)/suspended matter (SM) and aerosol size parameter (ASP) from ABI clear-sky spectral reflectances. The output is at 2-km spatial resolution and 5- and 15-minute temporal resolution during daytime. Due to the relatively weak aerosol signal and large uncertainties associated with surface reflectance, the current ABI algorithm does not attempt to do retrieval over bright surfaces, which include sun glint areas over water, desert, and bare soil surface over land. The primary retrieval product is AOD at 550 nm ( $\tau_{550}$ ), however AOD in five ABI channels (0.47, 0.64, 0.86, 1.61, and 2.25 µm) are also calculated based on the selected aerosol model. Aerosol size parameter is represented by two Ångström Exponents corresponding to two pairs of wavelengths (0.47/0.86 and 0.86/1.61µm). In addition, a single aerosol type over land, and a fine mode and a coarse mode aerosol type along with the corresponding fine-mode weight over ocean are retrieved. The aerosol products are intended for air quality and weather applications.

Tables 2-1, 2-2, 2-3, and 2-4 show the current F&PS requirements and product qualifiers for aerosol optical depth and size parameter.

Name	Geographic Coverage	Vertical Resolution	Horizontal Resolution	Mapping Accuracy	Measurement Range	Measurement Accuracy	Refresh Rate/Coverage Time Ontion (Mode 3)	Refresh Rate Option (Mode 4)	Vendor Allocated Ground Latency	Product Measurement Precision
Aerosol Optical Depth	C, FD	Total Column	2 km	l km	-1 <sup>*</sup> - 5 in optical depth	Based on Aerosol Optical Depth ranges: Over land: <0.04: 0.06 0.04 - 0.80: 0.04 > 0.80: 0.12 Over water: < 0.40: 0.02 > 0.40: 0.10	CON US:5 min Full Disk: 15 min	CON US:5 min Full Disk: 15 min	CONU S:50 sec Full Disk:1 59 sec	Based on Aerosol Optical Depth ranges: Over land: <0.04: 0.13 0.04 - 0.80: 0.25 > 0.80: 0.35 Over water: < 0.40: 0.15 > 0.40: 0.23

Table 2-1. GOES-R mission requirements for Aerosol Optical Depth.

\* Recommended to be changed to -0.05 instead of -1

Name	Temporal Coverage Qualifiers Geographic Coverage (G, H, C, M) User & Priority Name		Product Extent Qualifier	Cloud Cover Conditions Qualifier	Product Statistics Qualifier	
Aerosol Optical Depth	GOES-R	C, FD	2	degrees LZA (Threshold) and		Over specified geographic area

Table 2-2. Product qualifiers for Aerosol Optical Depth. LZA=local zenith angle.

Table 2-3. GOES-R mission requirements for Aerosol Particle Size.

Name	Geographic Coverage	Vertical Resolution	Horizontal Resolution	Mapping Accuracy	Measurement Range	Measurement Accuracy	Refresh Rate/Coverage Time Ontion (Mode 3)	Refresh Rate Option (Mode 4)	Vendor Allocated Ground Latency	Product Measurement Precision
Aerosol Particle Size	FD	Total Column	2 km	1 km	Fine/Coarse Angstrom exponent range: - 1 to +3	Fine/Coarse Angstrom exponent: 0.3 over ocean and land	Full Disk: 15 min	Full Disk: 5 min	Full Disk: 266 sec	0.15*

\* Recommended to relax from 0.15 to 0.6

Table 2-4. Product qualifiers for Aerosol Particle Size. LZA=local zenith angle.

Name	User & Priority	Geographic Coverage (G, H, C, M)	Temporal Coverage Qualifiers	Product Extent Qualifier	Cloud Cover Conditions Qualifier	Product Statistics Qualifier
Aerosol Particle Size	GOES-R	C, FD	-	degrees LZA (Threshold) and		Over specified geographic area

## 2.2 Instrument Characteristics

The Advanced Baseline Imager (ABI) on GOES-R has a total of 16 spectral bands in the visible, near-infrared and infrared spectral regions. The ABI spatial resolution is 2.0 km for the 1.38- $\mu$ m, 2.25- $\mu$ m and ten infrared (IR) spectral bands, and 0.5 km for the 0.64- $\mu$ m visible band. Spatial resolution of the other bands is 1.0 km. Table 2-5 lists these and the spectral characteristics of the instrument. ABI has on-board calibration of the reflected

solar channels with an expected absolute radiometric calibration accuracy of 5.0%, relative (one-sigma) calibration deviations (short-term repeatability) of 0.2%, calibrated radiances that correct for instrument degradation drift in radiance to 0.5% of the radiance. (Additional observations of lunar or stellar sources may be employed by NOAA operationally to attempt to improve long-term radiometric stability of the on-board calibration methodology over the ABI lifetime.) Details on the instrument design, calibration, and additional information on its characteristics are provided elsewhere, and not included in this ATBD. Table 2-5 also indicates which channels are currently used by the algorithm for aerosol retrieval.

Channel ID	Wavelength Microns	Hor. Res.	Upper and lower 50% response points (in microns)	Noise @ Ref.	Max. Level	Used
1	0.47	1km	0.45±0.01 - 0.49±0.01	300/1	100 %	✓ (land and internal test over water)
2	0.64	0.5km	0.59±0.01 - 0.69±0.01	300/1	100 %	✓ (land and water)
3	0.865	1km	0.8455±0.01 - 0.8845±0.01	300/1	100 %	✓ (water and internal test over land)
4	1.378	2km	1.3705±0.005 - 1.3855±0.005	300/1	100 %	✓ (internal test over land and water)
5	1.61	1km	1.58±0.01 - 1.64±0.01	300/1	100 %	✓ (water and internal test over land)
6	2.25	2km	2.225±0.01 - 2.275±0.01	300/1	100 %	✓ (land and water)

Table 2-5. Wavelengths, resolution, noise characteristics and use for aerosol retrieval of ABI bands.

7	3.90	2km	3.80±0.05 - 4.00±0.05	0.1 K	400 K	
8	6.185	2km	5.77±0.03 - 6.6±0.03	0.1 K	300 K	
9	6.95	2km	6.75±0.03 - 7.15±0.03	0.1 K	300 K	
10	7.34	2km	7.24±0.02 - 7.44±0.02	0.1 K	320 K	
11	8.5	2km	8.3±0.03 - 8.7±0.03	0.1 K	330 K	
12	9.61	2km	9.42±0.02 - 9.8±0.03	0.1 K	300 K	
13	10.35	2km	10.1±0.1 - 10.6±0.1	0.1 K	330 K	
14	11.2	2km	10.8±0.1 - 11.6±0.1	0.1 K	330 K	✓ (internal test over land and water)
15	12.3	2km	11.8±0.1 - 12.8±0.1	0.1 K	330 K	
16	13.3	2km	13.0±0.06 - 13.6±0.06	0.3 K	305 K	

Table 2-5 also lists the expected noise characteristics of the ABI in the various channels as given in the MRD. A detail analysis of the effect of instrument noise on the aerosol retrieval using various noise models is provided in Appendix A1.

## **3** ALGORITHM DESCRIPTION

This is the complete description of the algorithm at the current level of maturity.

#### 3.1 Algorithm Overview

The capabilities offered by ABI onboard GOES-R are similar to the multispectral observations currently provided by the Moderate Resolution Imaging Spectroradiometer (MODIS) flown on the NASA Earth Observing System (EOS) satellites Terra and Aqua, and by the Visible Infrared Imaging Radiometer Suite (VIIRS) flown on the Suomi National Polar-orbiting Partnership satellite, and to those that will be available from the Joint Polar Satellite System (JPSS). The ABI aerosol algorithm therefore heavily builds on the heritage of and the lessons learned from the MODIS [Remer et al., 2005, 2006; Levy

et al., 2007] and VIIRS [Vermote et al., 2006] aerosol algorithms. Separate algorithms are developed for retrieval over land and ocean due to the distinct surface properties and aerosol types.

Due to varying contribution of the surface to the satellite-observed reflectance and large variation in aerosol optical properties, aerosol retrieval is a complex problem. However, it is expected that observations of TOA reflectance at more than one wavelength can provide more information, and thus can reduce the number of unknowns and provide better constraints [King et al., 1978; Tanre et al., 1997]. In the ABI algorithm, this is achieved by the selection of appropriate aerosol models and by calculating and estimating the surface reflectance over ocean and land, respectively. Over land, surface reflectance is estimated by the dark-dense vegetation (dark-target) approach, in which surface reflectance in the visible spectrum is obtained from the shortwave infrared (SWIR) reflectance using predetermined relationships between these surface reflectances. To aid rapid retrieval of aerosol, look-up tables of spectral atmospheric (aerosols plus molecules) optical functions (reflectance, transmittances and spherical albedo) are pre-calculated for a wide range of geometries and typical aerosol models at standard surface pressure. Surface and atmospheric reflections are coupled following the VIIRS approach [Vermote et al., 2006]. The resulting calculated TOA reflectance is compared with observations to determine the optimal solution. Detailed explanation of the ABI aerosol retrieval algorithm is presented in the following chapters.

The geostationary platform offers observations at near constant local zenith angles, along with multiple looks of the same location in time over the course of a day. This feature has been exploited in remote sensing of aerosol and surface albedo in several algorithms [e.g., Knapp et al., 2005; Pinty et al., 2000; Thomas et al., 2007; Govaerts et al., 2010]. Many of these algorithms assume either that the aerosol amount is constant during the course of the day [Pinty et al., 2000], or require a priori information about the surface reflection properties [Thomas et al., 2007]. An algorithm that does not require some of these assumptions, and if developed further may replace the current ABI algorithm for retrieval over land, is being developed at the University of Maryland Baltimore County. This algorithm, which retrieves aerosol optical depth and surface bidirectional reflectance simultaneously even over bright surfaces, is briefly described in Section 6.3.1.

In principle, the multiple look with varying solar angles of a scene at a fixed local zenith angle from the geostationary platform may allow to partially "map out" the phase function. However, this would require the assumption of an unchanging aerosol type and amount. In addition, it would require very accurate navigation, and very accurate knowledge of the surface bidirectional reflectance. It is doubtful that these requirements can be satisfied at this time, so the current algorithm does not build on this theoretical possibility. Instead, the extensively tested and proven dark-target multi-channel algorithms developed for MODIS and VIIRS are used as heritage.

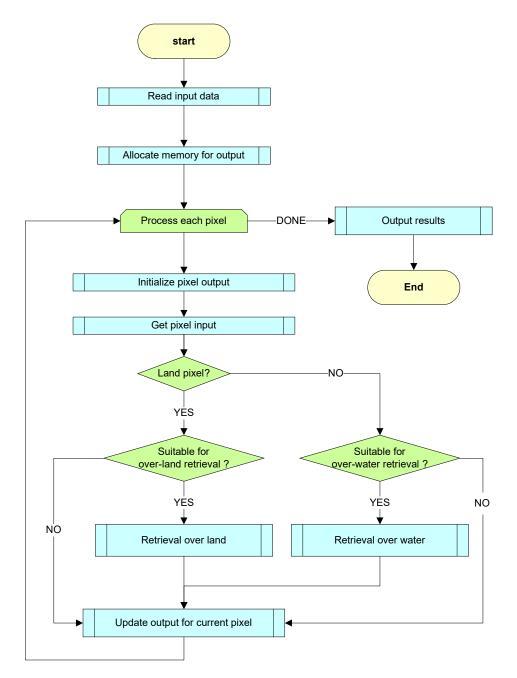


Figure 3-1. High level flowchart of the AOD retrieval illustrating the main processing sections.

## 3.2 Processing Outline

The processing outline of the AOD retrieval algorithm is summarized in Figure 3-1, which shows the major components of the algorithm. These components are: 1) Prepare input data for each 2 km "pixel"; 2) Determine retrieval eligibility and relevant algorithm to be used (land or water); 3) Perform aerosol retrieval; 4) Evaluate the retrieval quality and output the result.

## 3.3 Algorithm Input

This section describes the input needed to process the aerosol retrieval.

#### 3.3.1 Primary sensor data

Table 3-1 lists the primary sensor data used by the aerosol retrieval, including calibrated and geolocated level 1b reflectance (channels 1, 2, 4, 6 for land, and channels 2, 3, 4, 5, 6 for ocean) from ABI observations, geolocation information, and ABI sensor quality flags. Here it is assumed that (xsize, ysize) is the dimension at 2 km resolution.

Name	Туре	Description	Dimension
Ch1 reflectance	Input	Calibrated ABI channel 1	grid (xsize, ysize)
		reflectance at 2 km resolution	
Ch2 reflectance	Input	Calibrated ABI channel 2	grid (xsize, ysize)
		reflectance at 2 km resolution	
Ch3 reflectance	Input	Calibrated ABI channel 3	grid (xsize, ysize)
		reflectance at 2 km resolution	
Ch4 reflectance	Input	Calibrated ABI channel 4	grid (xsize, ysize)
		reflectance	
Ch5 reflectance	Input	Calibrated ABI channel 5	grid (xsize, ysize)
		reflectance at 2 km resolution	
Ch6 reflectance	Input	Calibrated ABI channel 6	grid (xsize, ysize)
		reflectance	
Ch14 brightness	Input	Calibrated ABI channel 14	grid (xsize, ysize)
temperature		brightness temperature	
Latitude	Input	Pixel latitude	grid (xsize, ysize)
Longitude	Input	Pixel longitude	grid (xsize, ysize)
Solar geometry	Input	ABI solar zenith and azimuth	grid (xsize, ysize)
		angles	
View geometry	Input	ABI local zenith and azimuth	grid (xsize, ysize)
		angles	
QC flags	Input	ABI quality control flags with	grid (xsize, ysize)
		input data	

The algorithm assumes the reflectance (r) is calculated from the calibrated radiance (L) by dividing  $\pi$  times the radiance by the product of the cosine of solar angle  $(\vartheta)$  and the extraterrestrial solar irradiance at the actual sun-earth distance (E):

$$r(\vartheta) = \frac{\pi L(\vartheta)}{\cos \vartheta E} . \tag{3.3.1}$$

The dimensions "xsize" and "ysize" correspond to the size of the (2-km) grid in the longitude and latitude directions, respectively. Their values are determined in the framework outside of the aerosol algorithm.

#### 3.3.2 Ancillary data

The algorithm requires three types of ancillary data: 1) ABI level 2 products (Table 3-2); 2) Global Forecast System (GFS) model data (Table 3-3); and 3) Non-ABI static data (Table 3-4).

ABI-derived cloud and snow/ice masks are needed to identify clear-sky snow/ice-free pixels for aerosol retrievals. The heavy aerosol mask (if available for cloud mask) is used to call-back (perform retrieval for) the opaque pixel identified as cloud by the external cloud mask. When the ABI snow/ice mask is not available, the Interactive Multisensor Snow and Ice Mapping System (IMS) is used. Land/sea mask is used to select the appropriate (land or ocean) algorithm for retrieval. The coastal mask, shallow inland water mask and shallow ocean mask are currently obtained from the land water mask. In case ABI-derived total precipitable water (TPW) and ozone data are not available or not valid, Global Forecast System (GFS) data are used instead. GFS model surface wind speed and direction over ocean is required for ocean surface reflectance calculation. The lower resolution model surface pressure is corrected to pixel-level pressure as:

$$P_{\text{pixel}} = P_{\text{model}} * \frac{e^{-H_{\text{digital}}}_{\& 8.24}}{e^{-H_{\text{model}}}_{\& 8.24}}$$
(3.3.2)

where  $P_{\text{pixel}}$  and  $P_{\text{model}}$  are actual pixel-level and model surface pressures;  $H_{\text{digital}}$  and  $H_{\text{model}}$  are high-resolution digital and low-resolution model surface elevations, respectively. A constant scale height of 8.24 km (adopted from the VIIRS ATBD) is assumed in this pressure correction.

Name	Туре	Description	Dimension
Cloud mask	input	ABI level 2 cloud mask data	grid (xsize, ysize)

Table 3-2. ABI dynamic ancillary input data

Heavy aerosol mask*	input	from ABI level 2 cloud mask data	grid (xsize, ysize)
Snow/Ice mask	input	ABI level 2 Snow/Ice mask data	grid (xsize, ysize)
TPW	input	ABI level 2 total precipitable water	grid (xsize, ysize)
Ozone	input	ABI level 2 ozone data	grid(xsize, ysize)

\* The current (as of February 2018) heavy aerosol mask contains only default values indicating no heavy aerosol. The AOD algorithm, however, still ingests the mask for future use in AOD retrieval and setting quality flags (see Tables 3-9 and 3-13).

Table 3-3. Non-ABI dynamic ancillary input data

Name	Туре	Description	Dimension
Model ocean surface wind speed & direction	input	Global Forecast System (GFS) data	grid (xsize, ysize)
Model surface pressure	input	Global Forecast System (GFS) data	grid (xsize, ysize)
Model surface height	input	Global Forecast System (GFS) data	grid (xsize, ysize)
Model total precipitable water	input	Global Forecast System (GFS) data	grid (xsize, ysize)
Model total ozone	input	Global Forecast System (GFS) data	grid (xsize, ysize)
Model snow/ice mask	input	Ice Mapping System (IMS) data	grid (xsize, ysize)

The spatial and temporal interpolation of GFS model data is a common procedure to many ABI algorithms, and is implemented at the framework level outside of the ABI aerosol algorithm; they are not described in this document.

Name	Туре	Description	Dimension
Land/Sea mask	input	Global land/water mask	grid(xsize, ysize)
Coastal mask	input	Global coastal mask	grid(xsize, ysize)
Shallow inland water mask	input	Global shallow inland water mask	grid(xsize, ysize)
Shallow ocean mask	input	Global shallow ocean mask	grid(xsize, ysize)
Surface elevation	input	Global digital elevation data	grid(xsize, ysize)

#### 3.3.3 Derived data

The derived data (Table 3-5) include pre-calculated LUTs and aerosol normalized and mass extinction coefficients.

There are two LUTs. The atmospheric LUT includes atmospheric reflectance, transmittance and spherical albedo in the ABI channels used for retrievals (three channels for land: 0.47, 0.64 and 2.25 $\mu$ m; four channels for ocean: 0.64, 0.86, 1.61 and 2.25  $\mu$ m). The sunglint LUT contains water direct-hemispheric reflectance and spherical albedo. Details of the LUTs are presented in Section 3.4.5.

Aerosol normalized extinction coefficients (ratio of the aerosol optical depth in ABI channels to that at 0.55  $\mu$ m) are used for calculating AODs at five ABI channels (0.47, 0.64, 0.86, 1.61, and 2.25  $\mu$ m) once AOD at 0.55  $\mu$ m ( $\tau_{0.55}$ ) and aerosol model are determined. Compared to the ocean aerosol models, land aerosol models are assumed to be dynamic, i.e., microphysical and optical properties vary with aerosol loading. As a result, extinction coefficients of land aerosol models are functions of  $\tau_{0.55}$ .

Aerosol mass extinction coefficients are needed to calculate suspended matter mass loading based on the retrieved  $\tau_{0.55}$ . These coefficients are adopted from the MODIS collection 5 algorithm since the same candidate aerosol models are used in the ABI retrieval. Similar to the normalized extinction coefficients, mass extinction of the land aerosol model depends on the aerosol loading and so it is a function of  $\tau_{0.55}$ . More information about aerosol column mass calculation is provided in section 3.4.4.

<b></b>		-	
Name	Туре	Description	Dimension
		atmospheric reflectance $\rho_{R+A}$ as a function of aerosol model, aerosol optical depth, ABI channel and scattering angle	(4, 20, 3,7727)* (9, 20, 4,7727)** (Nmodel, Ntau,Nchn,Nscaang)
Atmospheric LUT	Input	atmospheric transmittance $T_{R+A}$ as a function of aerosol model, aerosol optical depth, ABI channel and zenith angle	(4, 20, 3, 21)* (9, 20, 4, 21)** (Nmodel, Ntau,Nchn,Nzen)
		atmospheric spherical albedo $S_{R+A}$ as a function of aerosol model, aerosol optical depth, and ABI channel	(4, 20, 3)* (9, 20, 4)** (Nmodel, Ntau,Nchn)
Sunglint LUT	Input	water sunglint direct-hemispheric reflectance as a function of aerosol model, aerosol optical depth, ABI channel, solar zenith angle, local zenith angle, relative azimuth angle, and surface wind speed	(9, 20, 4, 21, 21, 40, 9) (Nmodel, Ntau,Nchn,Nsolzen, Nsatzen,Nwndspd)
		water spherical albedo as function of ABI channel and wind speed	(4, 9) (Nchn,Nwndspd)
Aerosol Normalized	Input	normalized aerosol extinction coefficient as a function of aerosol model, aerosol	(4, 20, 5)* (Nmodel, Ntau,Nchn)

Table 3-5. ABI derived input data

Extinction Coefficients		optical depth (land only) and ABI channel	(9 x 5)** (Nmodel, Nchn)
Aerosol Mass Extinction Coefficients	Input	Mass extinction coefficients for each aerosol model	(4,20) * (Nmodel, Ntau) (9,2) * (Nmodel, Npar)

\*: over land

\*\*: over ocean.

#### **3.4** Theoretical Description

This section describes the physics key to the aerosol retrieval over ocean and land. Description of the mathematics used by the retrieval, including all simplifications, approximations, and numerical methods, as well as the algorithm outputs are also presented.

The feasibility of aerosol retrieval from satellite-observed radiances is based on the fact that these radiances are affected by the physical and chemical properties of aerosols [e.g., King et al., 1978; Kaufman et al., 1990]. The wavelength bands of satellite sensors are selected to minimize gas and other contaminants to the aerosol signal. Because the ABI channels closely match those of MODIS and VIIRS, and because both algorithms have already been proven to work well, the ABI algorithm is designed to closely follow the approaches used with these sensors [Remer et al., 2005, 2006; Levy et al., 2007; Vermote et al., 2006; Jackson at al., 2013]. Just like the MODIS and VIIRS algorithms, the ABI algorithm retrieves the aerosol optical depth and the most likely aerosol model simultaneously from radiances observed in the visible and near infrared channels. The assumption is that the contribution of the ocean surface can be accurately computed, and the land surface reflectance can be estimated. Therefore there are two separate algorithms: one for ocean and one for land.

Aerosol retrievals are also affected by the presence of various "contaminants" in the pixel that can degrade the quality of aerosol retrievals. These include snow for land, and glint and turbid water for ocean [e.g., Remer et al., 2005, 2006]. How the ABI algorithm deals with these contaminants is described in Sections 3.4.1.6 and 3.4.2.6.

# 3.4.1 Physical and mathematical description for aerosol optical depth retrieval over ocean

#### 3.4.1.1 Strategy

The algorithm for aerosol retrieval over ocean is based on Tanré et al. (1997) and its implementation in the VIIRS algorithm [Vermote et al., 2006]. However, the aerosol models used by the algorithm are from the MODIS Collection 5 algorithm [Remer et al.,

2005, 2006; Levy et al., 2007]. ABI channels 2, 3, 5 and 6, for which surface reflection can be estimated without information on ocean color, are used [Vermote et al., 2006]. Thus, for example, ABI channel 1 (0.47 $\mu$ m) is not included due to the large uncertainty in water leaving radiance.

It is assumed that the surface reflectance of water can be modeled with sufficient accuracy as shown by Cox and Munk [1954]. Therefore, the essence of the multi-channel aerosol algorithm over water is the simultaneous retrieval of optical depth and aerosol model by matching calculated and observed TOA reflectances in selected ABI channels. The contribution of aerosol to the TOA reflectance is approximated by a linear combination of two aerosol modes corresponding to a fine and a coarse mode of the size distribution with a fine mode weight [e.g. Tanré et al., 1997]. Since an exact match of TOA reflectance in all selected channels is nearly impossible, the algorithm uses ABI channel 3 (0.86 µm) as the principal channel, where the aerosol optical depth at 550 nm ( $\tau_{550}$ ) and fine-mode weight  $(\eta)$  retrieval is performed to match the observed TOA reflectance. The 0.86-µm channel is chosen because of its negligible underwater reflectance, while the contributions from the fine and coarse aerosol modes are still significant. The sum of squared differences of calculated and observed reflectances in other channels is calculated as the residual for the judgment of the degree of match, and the minimum residual is considered as the 'best' match. The process of checking for minimum residual is repeated and the solution that gives the minimum residual is chosen for the retrieval of  $\tau_{550}$  and  $\eta$ . AOD at other wavelengths are determined by using the spectral dependence of aerosol optical properties unique to that aerosol model, which is included in the pre-calculated LUT.

Surface reflection, including water leaving radiance, whitecaps and sun glint direct reflection (Section 3.4.1.5), and atmosphere-surface coupling (Section 3.4.1.3) are explicitly calculated in the algorithm. Dependence of ocean surface reflectance on surface wind is incorporated, which can be significant at mid-high latitude where relatively large wind speeds dominate. This is in contrast to the MODIS collection 5 aerosol algorithm that assumed a constant wind speed of 6 m/s [Remer et al., 2005].

#### 3.4.1.2 Aerosol models

Over ocean, the aerosol model is represented by a combination of fine-mode and coarse mode aerosols. The four fine and five coarse mode models adopted from MODIS [Remer et al., 2005, 2006; Levy et al., 2007] are summarized in Table 3-6. The size distribution for these aerosols is assumed to be log-normal:

$$\frac{dN(r)}{d\ln r} = \sum_{i=1}^{2} \frac{N_0}{\sqrt{2\pi} \ln \sigma_{g,i}} \exp \left[ -\frac{\left(\ln r - \ln r_{g,i}\right)^2}{2\left(\ln \sigma_{g,i}\right)^2} \right],$$
(3.4.1)

where N(r) is the number density corresponding to particles of radii within (r, r+dr),  $r_{g,i}$  is the median radius, and  $\sigma_{g,i}$  is the associated standard deviation. Microphysical properties of the aerosol models are listed in Table 3-6, which are derived from the prescribed size distribution and refractive index from MODIS aerosol models [Remer, et al, 2006]. The aerosol effective radius (microns) is an area weighted mean radius and defined as

$$r_{eff} = \frac{\int_{0}^{\infty} r^3 N(r) dr}{\int_{0}^{\infty} r^2 N(r) dr},$$
 where *r* is the particle radius, and *N*(*r*) the particle size distribution

(number of particles per cm<sup>2</sup> with radius in the range *r* and *r*+*dr*). For calculation of aerosol optical properties, integration of aerosol size distribution (Eq. 3.4.1) is performed within the radius range of 0.05 to 15.0  $\mu$ m following the Mie calculation in the 6S radiative transfer model (RTM) [Kotchenova et al., 2006; 2007].

Table 3-6. Microphysical properties of ocean aerosols (Fine modes: F1-F4; Coarse modes: C1-C5) used in the ABI algorithm (refractive index, number median  $(r_g)$ , standard deviation  $(\sigma_g)$ , and effective radius  $(r_{eff})$ ).

Aerosol model	Refractive index Wavelength (μm)				$r_{g}$	$\sigma_{_g}$	r <sub>eff</sub>		
model	0.47	0.64	0.86	1.38	1.61	2.26	_	-	
F1	1.45- 0.0035i	1.45- 0.0035i	1.45- 0.0035i	1.44- 0.005i	1.43- 0.01i	1.40- 0.005i	0.07	1.49182	0.10
F2	1.45- 0.0035i	1.45- 0.0035i	1.45- 0.0035i	1.45- 0.005i	1.43- 0.01i	1.40- 0.0050i	0.06	1.82212	0.15
F3	1.40- 0.002i	1.40- 0.002i	1.40- 0.002i	1.40- 0.0035i	1.39- 0.005i	1.36- 0.003i	0.08	1.82212	0.20
F4	1.40- 0.002i	1.40- 0.002i	1.40- 0.002i	1.40- 0.0035i	1.39- 0.005i	1.36- 0.003i	0.10	1.82212	0.25
C1	1.35- 0.001i	1.35- 0.001i	1.35- 0.001i	1.35- 0.001i	1.35- 0.001i	1.35- 0.001i	0.40	1.82212	0.98
C2	1.35- 0.001i	1.35- 0.001i	1.35- 0.001i	1.35- 0.001i	1.35- 0.001i	1.35- 0.001i	0.60	1.82212	1.48
C3	1.35- 0.001i	1.35- 0.001i	1.35- 0.001i	1.35- 0.001i	1.35- 0.001i	1.35- 0.001i	0.80	1.82212	1.98
C4	1.53- 0.003i	1.53-0.0i	1.53-0.0i	1.46-0.0i	1.46- 0.001i	1.46-0.0i	0.60	1.82212	1.48
C5	1.53- 0.003i	1.53-0.0i	1.53-0.0i	1.46-0.0i	1.46- 0.001i	1.46-0.0i	0.50	2.2255	2.50

#### 3.4.1.3 Calculation of TOA reflectance

Calculation of TOA reflectance follows that in the VIIRS ATBD [Vermote et al., 2006], which itself is based on the formulation in the Second Simulation of the Satellite Signal, 6S radiative transfer model [Vermote et al., 1997, Kotchenova et al., 2006; 2007]. According to this formulation, the spectral reflectance at the satellite level ( $\rho_{toa}$ ) is the combination of two components  $\rho_{atm}$  and  $\rho_{surf}$  originating, respectively, in the atmosphere and at the surface.

$$\rho_{toa} = \rho_{atm} + \rho_{surf} \,. \tag{3.4.2}$$

The atmospheric contribution is due to reflection, scattering by molecules and aerosols and absorption by aerosols and gases. The surface contribution comes from the multiple reflection of radiation between the surface and the atmosphere that is subsequently attenuated by the atmosphere as it travels upward to the satellite.

To facilitate the calculation of atmospheric reflection with varying gaseous amount and surface pressure, gas absorption, aerosol and Rayleigh scattering are decoupled in a layered model atmosphere. In this model, radiation produced in a layer with molecular scattering, aerosol extinction, and water vapor absorption is attenuated by absorption in the top layer by ozone, O<sub>2</sub>, CO<sub>2</sub>, N<sub>2</sub>O, and CH<sub>4</sub>. Ignoring the interaction between aerosol and Rayleigh scattering, the atmospheric contribution to TOA reflectance is computed as:

$$\rho_{atm} = T^{O_3} T^{O_g} \bigg[ (\rho_{R+A} - \rho_R(P_0)) T^{\frac{1}{2}H_2O} + \rho_R(P) \bigg], \qquad (3.4.3)$$

where,  $T^{O_3}$  is the transmittance from ozone absorption;  $T^{og}$  is the transmittance from gas absorption other than ozone and water vapor;  $T^{\frac{1}{2}H_2O}$  is the transmittance from half column water vapor absorption;  $\rho_{R+A}$  is the path reflectance by aerosols and molecules at standard surface pressure;  $\rho_R(P_0)$  is the Rayleigh reflectance from molecular scattering at standard surface pressure;  $\rho_R(P)$  is the Rayleigh reflectance from molecular scattering at the actual surface pressure P. Here,  $\rho_{R+A}$  is pre-calculated and stored in the atmospheric LUT (see section 3.4.5.1), while gas transmittances T and Rayleigh reflectance  $\rho_R$  are analytically modeled (see sections 3.4.6 and 3.4.7). Rayleigh reflectance  $\rho_R$  is calculated at the given local surface pressure and at standard pressure, respectively (see section 3.4.7). Note that the channel index has been dropped from the notation for convenience in the discussion.

The reflectance of ocean surface is modeled as the sum of (bi-directional) sunglint reflection, (Lambertian) underwater reflection and whitecap reflection (see section 3.4.1.5). Interaction between the atmosphere and the surface is decomposed into the sum of six terms in Eq. (3.4.4) corresponding to the contributions from (1) Lambertian reflection from underwater and whitecaps; (2) directional sunglint reflection without atmospheric scattering; (3) diffuse downward radiation reflected by the surface and transmitted to the sensor without scattering; (4) direct downward radiation reflected by surface and scattered back to the sensor; and (6) radiation reflected by the surface more

than once. For efficient calculations, a look-up table (see section 3.4.5.2) was generated using the 6S radiative transfer model [Vermote et al., 1997] for the necessary terms (e.g.,  $\overline{\rho_{sgt}}$ ,  $\overline{\rho_{sgt}}$  and  $\overline{\rho_{sgt}}$ ). The diffuse transmittance is calculated by subtracting the direct transmittance from the total transmittance. The glint contribution is weighted by the foamfree fraction (1-W), where W is the fraction covered with whitecap and calculated as a function of wind speed (ws), 2.95\*10<sup>-6</sup> ws <sup>3.52</sup> [Koepke, 1984]. All terms are calculated for the central wavelength of the ABI channels.

$$\rho_{surf} = T^{O_3} T^{og} T^{H_2O} \begin{bmatrix} T^{\downarrow}_{R+A} T^{\uparrow}_{R+A} \frac{\rho_{w+wc}}{1 - S_{R+A} \rho_{w+wc}} + (1 - W) (t^{dir\downarrow}_{R+A} t^{dir\uparrow}_{R+A} \rho_{sgt} + t^{dif\downarrow}_{R+A} t^{dir\uparrow}_{R+A} \overline{\rho_{sgt}} \\ + t^{dir\downarrow}_{R+A} t^{dir\uparrow}_{R+A} \overline{\rho_{sgt}} + t^{dif\downarrow}_{R+A} t^{dir\uparrow}_{R+A} \overline{\rho_{sgt}} + T^{\downarrow}_{R+A} T^{\uparrow}_{R+A} \frac{S_{R+A} (\overline{\rho_{sgt}})^2}{1 - S_{R+A} \overline{\rho_{sgt}}} \end{bmatrix} , \quad (3.4.4)$$

$$t_{R+A}^{uv} = e^{-t_{R+A}^{uv}\cos(\theta_s)}, \qquad (3.4.5)$$

$$t_{R+A}^{dir_{+}} = e^{-\tau_{R+A}/\cos(\theta_{v})}, \qquad (3.4.6)$$

$$t_{R+A}^{aly} = T_{R+A}^* - t_{R+A}^{alv}, \tag{3.4.7}$$

$$t_{R+A}^{dij+} = T_{R+A}^{+} - t_{R+A}^{dir+}, (3.4.8)$$

$$\tau_{R+A} = \tau_A + \tau_R(P), \qquad (3.4.9)$$

where,  $T_{R+A}^{\downarrow}$  is the total (direct and diffuse) downward atmospheric transmission;  $T_{R+A}^{\uparrow}$  is the total (direct and diffuse) upward atmospheric transmission;  $t_{R+A}^{dir\downarrow}$  is the direct downward atmospheric transmission;  $t_{R+A}^{dir\uparrow}$  is the direct upward atmospheric transmission;  $t_{R+A}^{dir\downarrow}$  is the diffuse downward atmospheric transmission;  $t_{R+A}^{dir\uparrow}$  is the diffuse upward atmospheric transmission;  $S_{R+A}$  is the atmospheric spherical albedo;  $\rho_{w+wc}$  is the surface Lambertian reflectance from underwater and whitecaps;  $\rho_{sgt}$  is the sunglint directional reflectance;  $\overline{\rho_{sgt}}$  is the normalized integral of the downward irradiance by the sunglint directional reflectance;  $\overline{\rho_{sgt}}$  is the reciprocal quantity of  $\overline{\rho_{sgt}}$  for the upward coupling;  $\overline{\rho_{sgt}}$  is approximated as the sunglint spherical albedo;  $\theta_s$  is the solar zenith angle;  $\theta_v$  is the local zenith angle;  $\tau_{R+A}$  is the total column optical thickness of molecules and aerosols;  $\tau_R(P)$ is the Rayleigh optical depth at local actual pressure P, and  $\tau_A$  is the retrieval unknown (the aerosol optical depth). Note that  $\tau_R(P)$  and  $\tau_A$  should use the values for the specific wavelength.  $T_{R+A}^{\downarrow}$ ,  $T_{R+A}^{\uparrow}$ , and  $S_{R+A}$  are obtained from the atmospheric look-up table, and require adjustment for the actual surface pressure following Eq. (3.4.35) and Eq. (3.4.36) in section 3.4.6.  $\overline{\rho_{sgt}}$ ,  $\overline{\rho_{sgt}}$ , and  $\overline{\rho_{sgt}}$  are obtained from the ocean surface reflectance lookup table (see Appendix B).

#### 3.4.1.4 Aerosol retrieval algorithm over ocean

The retrieval algorithm assumes that aerosol reflectance  $\rho_{\lambda}^{t}$  for a given  $\tau_{550}$  can be approximated with a linear combination of contributions from one fine  $(\rho_{\lambda}^{f})$  and one coarse  $(\rho_{\lambda}^{c})$  aerosol modes with a fine-mode weight  $\eta$  [Wang and Gordon, 1994; Kaufman and Tanre, 1996],

$$\rho_{\lambda}^{t}(\tau_{550}) = \eta \rho_{\lambda}^{f}(\tau_{550}) + (1 - \eta) \rho_{\lambda}^{c}(\tau_{550}).$$
(3.4.10)

In the retrieval, the algorithm searches for the pair of fine and coarse modes, along with the fine mode weight ( $\eta$ ) and corresponding  $\tau_{550}$  that give the best match of TOA reflectance in multiple ABI channels between calculations and observations.

Specifically, there are two levels of iteration and selection involved. The first iteration is on the combination of candidate fine and coarse modes, which are predetermined and built into the lookup table. In the current algorithm, there are four (fine mode) by five (coarse model) combination pairs.

The second iteration (searching for  $\eta$  for any given pair of fine and coarse aerosol modes) uses bisection (interval halving), which repeatedly divides the fine-mode weight range in half and searches for the subinterval that includes the 'best' fit  $\eta$  with minimum residual. Ranges of the fine mode weight, starting with the full range of 0-1, are repeatedly bisected, AODs are retrieved and residuals are calculated. Altogether ten bisection steps are performed, regardless of measurement uncertainty. In each step, the interval that results the smallest residual in the previous step is selected for the bisection. The process starts with dividing the range of  $\eta$  between 0 and 1 into four equal subintervals with ranges of 0.00-0.25, 0.25-0.50, 0.50-0.75, and 0.75-1.00. AODs are retrieved for the five boundary values of  $\eta$  (0, 0.25, 0.5, 0.75 and 1), and residuals are calculated. The smallest residual is identified among the five residuals and the subinterval containing the smallest residual is selected for further processing (bisection). So, for example, if the residuals corresponding to the five starting values of  $\eta$  are  $R_{0.0}$ ,  $R_{0.25}$ ,  $R_{0.5}$ ,  $R_{0.75}$  and  $R_{1.0}$ , and if  $R_{0.0}$  (or  $R_{0.25}$ ) is the smallest residual then the two intervals 0.00-0.25 and 0.25-0.50 are bisected leading to another five values of  $\eta$  (0.0, 0.125, 0.25, 0.375, 0.5). AODs and residuals are calculated for these  $\eta$  values. (Note that retrievals are already performed for the  $\eta$  values of 0, 0.25 and 0.5 in the previous step, so in reality they need to be done only for the  $\eta$  values of 0.125 and 0.375.) If  $R_{0.5}$  is the smallest then the middle two subintervals (0.25-0.5 and 0.5-0.75) are used. If  $R_{0.75}$  (or  $R_{1.0}$ ) is the smallest the upper two subintervals (0.5-0.75 and 0.75-1.0)

are used. The process is repeated ten times and usually reaches 0.1% accuracy, and the  $\eta$  (and AODs) corresponding to the smallest residual is selected as the solution. If two or more residuals are identical within machine precision, the first one in the sequence (the one corresponding to the smallest  $\eta$ ) is selected. The determination of  $\tau_{550}$  for any specific aerosol model (combination of fine and coarse modes with known  $\eta$ ) is performed by matching the calculated TOA reflectance at 0.86 µm with the measurement. Extrapolation is allowed and flagged for  $\tau_{550} > 5$  or  $\tau_{550} < 0$  when  $\tau_{550}$  is outside of the AOT550 range tabulated in LUT. The best match is determined by comparing the residuals that are calculated as the sum of squared differences between calculated ( $\rho_{\lambda}^{cal}$ ) and observed ( $\rho_{\lambda}^{obs}$ ) TOA reflectances in the ABI channels 2, 5 and 6 (0.64, 1.61, and 2.25 µm):

$$residual = \sum_{i=1}^{n} (\rho_{\lambda}^{cal} - \rho_{\lambda}^{obs})^2, \qquad (3.4.11)$$

where n = 3, the number of channels used for calculating the residual, and  $\rho_{\lambda}^{cal}$  corresponds to  $\rho_{toa}$  in Eq.(3.4.2)

Once the final solution of aerosol model and corresponding  $\tau_{550}$  are determined, AODs in the five ABI channels (channels 1,2,3,5, and 6) are calculated by the unique spectral dependence of aerosol extinction coefficient for the retrieved combination of fine and coarse mode aerosol models and fine mode weight  $\eta$ . That is, the optical depth at wavelength  $\lambda$  is calculated as  $\tau_{\lambda,fine/coarse} = n_{ext,\lambda,fine/coarse} \times \tau_{550}$  for the retrieved fine and coarse mode aerosol models, respectively, where  $n_{ext,\lambda}$  is the normalized extinction coefficient at wavelength  $\lambda$  included in the LUT for each fine and coarse mode aerosol model. The final AOD at wavelength  $\lambda$  is calculated as  $\tau_{\lambda} = \tau_{\lambda,fine} \times \eta + \tau_{\lambda,coarse} + (1-\eta)$ .

#### 3.4.1.5 Calculation of ocean surface reflectance

As discussed in Section 3.4.1.3, the reflectance of ocean surface is modeled as the sum of bi-directional sun-glint, Lambertian dark underwater and whitecap reflections. The calculation for each of these reflection terms contains wavelength-specific coefficients. These coefficients were derived for the visible-to-near-infrared ABI channels using the 6S RTM, where the sunglint bi-directional reflectance distribution function (BRDF) is calculated from the Cox and Munk model [Cox and Munk, 1954].

Water and whitecap reflectance  $\rho_{_{W+WC}}$  is calculated as

$$\rho_{w+wc} = (1 - \rho_{wc})\rho_w + \rho_{wc}, \qquad (3.4.12)$$

$$\rho_{wc} = \rho_{wc-eff} \cdot 2.95 \times 10^{-6} [ws]^{3.52} \tag{3.4.13}$$

where  $\rho_w$  and  $\rho_{wc}$  are reflectances from underwater and whitecap respectively, ws is the wind speed in m s<sup>-1</sup>.  $\rho_{wc}$  is the product of an effective reflectance  $\rho_{wc-eff}$  and whitecap coverage [Koepke, 1984]. For simplicity, chlorophyll concentration is fixed (0.4 mg m<sup>-3</sup>). Dependence of water reflectance on wind speed is week, and the wind-speed dependence of whitecap reflectance is accounted for by the wind-speed dependent whitecap coverage in Eq. (3.4.13). Table 3-7 contains the channel-dependent constants for  $\rho_w$  and  $\rho_{wc-eff}$ .

ABI Channel (wavelength: μm)	$ ho_{\scriptscriptstyle wc-e\!f\!f}$	$ ho_w$
2 (0.64)	0.2200	<mark>0.00131</mark>
3 (0.86)	0.1982	0.0
5 (1.61)	0.1195	0.0
6 (2.25)	0.0471	0.0

Table 3-7. Whitecap effective reflectance and water reflectance

Calculation of sunglint directional reflectance  $\rho_{sgt}$  is adopted from the corresponding 6S subroutine [Vermote et al., 1997; Cox and Munk, 1954]. It requires inputs of wind speed WS (in m s<sup>-1</sup>), index of refraction (n<sub>r</sub>, n<sub>i</sub>) and extinction coefficient of the sea water, solar zenith angle  $\theta_s$ , local (view) zenith angle  $\theta_v$ , and sun, local and wind azimuth angles  $\phi_s, \phi_v, \phi_w$  (clockwise from local North). The index of refraction and extinction coefficient (Table 3-8) of sea water are calculated from the 6S RTM assuming a constant salinity of 34.3 ppt. Details of the sunglint directional reflectance calculation are given in Appendix B.

Table 3-8. Seawater index of refraction and extinction coefficient for ABI bands

ABI Channel (wavelength: μm)	Nr	Ni
2 (0.64)	1.3374739	0.0
3 (0.86)	1.3344265	0.0000003
5 (1.61)	1.3227725	0.0000868
6 (2.25)	1.2984004	0.0004302

#### 3.4.1.6 Internal Tests and Quality Control

Producing a high quality AOD product requires an effective process to screen out pixels that do not satisfy the assumptions applied in the retrieval. In addition to cloud, snow, coastal and shallow inland water/ocean external masks, several simple internal tests are developed to identify unfavorable retrieval conditions:

- 1) Internal cloud test:  $\rho_{0.86\,\mu m}^{obs} > 0.3$  is used to screen out thick cloud;
- 2) Internal cirrus test: Cirrus is identified if  $\rho_{1.38\mu m}^{obs} > 0.018$ ;
- 3) Internal inhomogeneity test: Standard deviation ( $\sigma_{2.25\,\mu m}^{3\times3}$ ) of 2.25- $\mu$ m reflectances  $\rho_{2.25\,\mu m}^{obs}$  is calculated for 3x3 2-km pixels centered on each ocean pixels. A pixel is deemed as spatially inhomogeneous if  $\sigma_{2.25\,\mu m}^{3\times3}$  is larger than 0.008;
- 4) <u>Internal sea ice test</u>: Sea ice is detected if  $\frac{\rho_{0.64\mu m}^{obs} \rho_{1.61\mu m}^{obs}}{\rho_{0.64\mu m}^{obs} + \rho_{1.61\mu m}^{obs}} > 0.4 \text{ and } \rho_{0.64\mu m}^{obs} > 0.2$

and  $\rho_{0.86\,\mu m}^{obs} > 0.17$  and the brightness temperature at 11  $\mu$ m is lower than 275K;

- 5) <u>Internal shallow water test:</u> Retrieval over shallow water is avoided if  $f''(\rho_{0.64\mu m}^{obs}) < -0.07$ . Here  $f''(\rho_{0.64\mu m}^{obs})$  is a parameter proportional to the second derivative of the spectral reflectance at channel 0.64µm, and is calculated as  $f''(\rho_{0.64\mu m}^{obs}) = 2.2\rho_{0.47\mu m}^{obs} 3.9\rho_{0.64\mu m}^{obs} + 1.7\rho_{0.86\mu m}^{obs}$ .
- 6) <u>Internal sunglint test:</u> Retrieval over sunglint region is avoided if the glint angle is less than 40°. The glint angle is defined as the angle between the observing vector and the specular reflection direction, and calculated as

 $\theta_g = \cos^{-1}((\cos\theta_s\cos\theta_v) - (\sin\theta_s\sin\theta_v\cos\phi))$ , where  $\phi$  is the relative azimuth angle.

Based on the input masks, internal tests as well as the retrieval residual, retrievals are categorized into four quality levels: no retrieval; low; medium; and high quality. The criteria used for assigning quality are listed in Table 3-9. In general, the high quality retrievals are recommended for quantitative applications due to their better overall performance; however, the lower quality retrievals also have their merit for qualitative examination of local episodic events due to their greater spatial coverage.

Quality Level	Criteria		
No Retrieval	<ol> <li>Cloudy: external cloud mask is cloudy and any internal cloud reflectance, cirrus or inhomogeneity test fails;</li> <li>Sea ice (external mask or internal test);</li> <li>Shallow water (internal test);</li> <li>Sunglint (internal test)</li> </ol>		
Low	<ol> <li>Out of AOD range (-0.05, 5.0);</li> <li>Solar zenith angle &gt; 80°;</li> </ol>		

Table 3-9: Criteria used for assigning retrieval quality over water.

	3) Satellite zenith angle $> 60^{\circ}$ ;
	<ul><li>4) Failed internal cloud test, but external cloud mask is clear or</li></ul>
	probably clear;
	5) Failed internal cirrus test, but external cloud mask is clear or probably clear;
	6) External cloud mask is cloudy or probably cloudy, but passed
	internal tests, and not heavy aerosol;
	7) Coastal area (from external coastal mask);
	8) Shallow inland water (external shallow inland water mask);
	9) $\sigma_{2.25\mu m}^{3\times3} > 0.008;$
	10) Retrieval residual $> 0.3$
	1) Adjacent to cloudy pixel;
	2) Adjacent to snow pixel (within 3-pixel distance)
Medium	3) $\sigma_{2.25\mu m}^{3\times3} > 0.002;$
Iviculuiii	4) Retrieval residual $> 0.25$ ;
	5) Shallow ocean (external shallow ocean mask)
	6) External cloud mask is 'probably clear';
High	Remaining retrievals

Note that after setting the quality flag to low out-of-range AOD values are re-set to the appropriate boundaries of the valid range. These truncated values are the ones that are reported in the final AOD product.

### 3.4.1.7 Sensitivity study

The quality of aerosol retrieval can be strongly affected by the uncertainties in the TOA radiances (for example, due to calibration, cross talk, polarization sensitivity, etc.). In multi-channel aerosol retrievals, estimation of these effects is not straightforward owing to the complex interdependencies of channel radiances and assumptions. As part of algorithm testing, numerical tests were designed to investigate the sensitivity of aerosol retrieval to ABI radiance uncertainties.

For these tests, TOA ABI radiances are simulated by the forward 6S RTM for a wide range of geometries and aerosol conditions. Table 3-10 lists these varying parameters as inputs to the simulations. A constant water vapor (2 cm) and ozone content (380 Dobson units), and surface wind condition (6 m/s, westerly) is assumed in the simulation (and in the subsequent inversion). Among the 840,000 cases resulting from the combinations of input values listed in Table 3-10, there are 423,640 unique tests that are outside of the sunglint area (glint angle  $\theta_g > 40^\circ$  and that are used for in following evaluation.

Table 3-10. Geometry and aerosol conditions co	overed by the sensitivity tests
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Parameters Dir	nsion Values
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	cosine of solar zenith angle	10	from 0.4 to 1.0 with a constant interval of 1/15
Geometry	cosine of local zenith angle	10	from 0.4 to 1.0 with a constant interval of 1/15
	relative azimuth angle	10	from 0° to 180° with a constant interval of 20°
Aerosol	fine Mode	4	four fine modes same as those in the retrieval algorithm
Models	coarse Mode	5	five coarse modes same as those in the retrieval algorithm
	fine mode weight	6	0, 0.2, 0.4, 0.6, 0.8, 1.0
Aerosol optical depth at 0.55µm		7	0.1, 0.2, 0.4, 0.6, 0.8, 1.0, 1.5

To simulate the calibration uncertainty, the ABI radiances in all channels were perturbed at 3% and 5% levels, which included 1) random noise without systematic bias; 2) positive and negative systematic biases; and 3) systematic biases plus random noise. Variation in channel-to-channel calibration was also simulated by adding a 3% bias to the individual channels. Altogether, there were 14 types of perturbations with 423,640 retrieval cases for each type. Outputs from the retrievals with perturbed radiances were compared with unperturbed retrieval results to evaluate the sensitivity of the algorithm to the calibration uncertainties.

The general results for the 14 types of sensitivity tests are displayed in Figure 3-2, where the averaged uncertainty and standard deviation of retrieved  $\tau_{0.55\mu m}$  and aerosol fine mode weight (FMW), as well as the percentage of misidentification of aerosol models are shown. The tests with perturbations in all ABI channels (top panel in Figure 3-2), indicate that the random noise does not introduce a bias in the retrieved  $\tau_{0.55\mu m}$  and FMW; however, the large standard deviations indicate large variability. Large positive systematic errors in all channel radiances lead to the overestimation of  $\tau_{0.55\mu m}$  and FMW, while an underestimation of  $\tau_{0.55\mu m}$  and FMW, while an underestimation

occurs with negative perturbations. The relative uncertainties of retrieved  $\tau_{\rm 0.55\mu m}$  (defined

as  $\frac{perturbed - unperturbed}{unperturbed}$ ) are about 5% and 9% for the radiance biases at 3% and 5%

levels, respectively. Associated FMW uncertainties are in the range of 0.01 to 0.04.

Perturbation of TOA reflectance in a single channel also exhibits significant influence on aerosol retrievals (last 4 columns of top panel in Figure 3-2). Increasing the TOA reflectance by 3% in the reference channel (0.86 µm) results in a similar positive bias (~3%) in the retrieved  $\tau_{0.55\mu m}$ , while the averaged uncertainty of FMW is small (< 0.01). When the perturbation is applied to the other channels used for residual calculation, it changes the spectral shape of reflectance, therefore different aerosol models can be selected, which in turn, affects the retrieved  $\tau_{0.55\mu m}$  even when the reference channel is

unperturbed. Such effect is seen when the TOA reflectance in the red channel (0.64  $\mu$ m) is enhanced by 3%. This change in spectral shape favors fine mode aerosol selection; as a result, the retrieved average FMW is increased by 0.025 and the corresponding  $\tau_{0.55\mu m}$ increased by 2%. On the other hand, increasing the TOA reflectance in the near-infrared channel (1.61  $\mu$ m) by 3% favors coarse mode aerosols, and the retrieved FMW decreases by 0.02 while  $\tau_{0.55\mu m}$  increases by 3%. As for the SWIR channel (2.26  $\mu$ m), it appears that the effect on the aerosol retrieval is minimum; however, the averaged uncertainty of retrieved  $\tau_{0.55\mu m}$  is about 1.6%, which cannot be deemed insignificant.

As seen from Figure 3-2, aerosol model selection is very sensitive to the perturbation of reflectance as the average rate of misidentification is above 40% and 50% for the 3% and 5% perturbation in all channels. Misidentification can be greater than 80% when the individual channel perturbation changes the spectral shape of TOA reflectance.

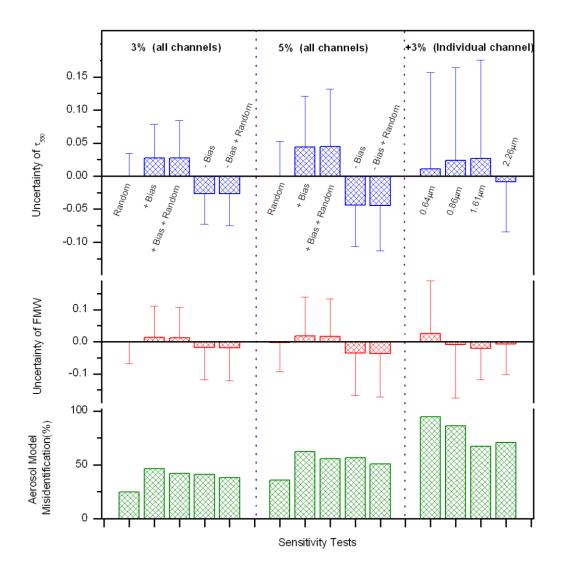


Figure 3-2. Average uncertainties in the retrieved aerosol optical depth at 0.55  $\mu$ m, fine- mode weight and percentage of model misidentification for all sensitivity tests.

It should be noted that the uncertainties calculated from these tests mask the detailed complex dependencies on the geometry, aerosol type and loading. An example of angular dependence is shown in Figure 3-3. In this case, the TOA reflectance at 1.61  $\mu$ m was increased by 3%, applied to the fine mode #2 and coarse mode #1 with 0.4 FMW and  $\tau_{0.55\mu m} = 0.2$ . The averaged uncertainty of retrieved  $\tau_{0.55\mu m}$  is -0.006, while the maximum  $\Delta$ 

 $\tau_{0.55\mu m}$  can be as large as 0.014 and the minimum can reach -0.033. Similarly, the averaged  $\Delta$  FMW is -0.039, while the maximum is 0.21 and minimum is -0.20.

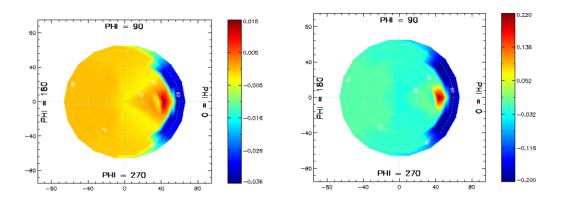


Figure 3-3. Angular dependence of the uncertainty of retrieved  $\tau_{550}$  (left) and FMW (right) for one case: increasing TOA reflectance at 1.61 µm by 3%, applied to the second fine mode #2 and coarse mode #1 with 0.4 FMW and  $\tau_{550} = 0.2$ . Solar zenith angle is 42.83°. In the figure, local zenith angle increases in the radial direction; PHI represents the relative azimuth angle.

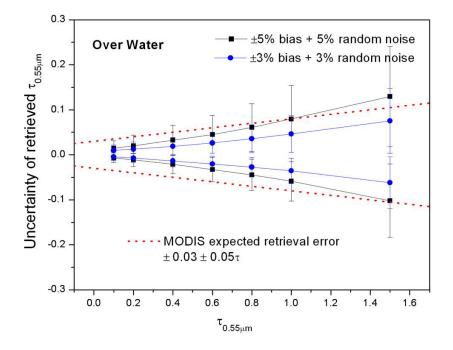


Figure 3-4. Uncertainty of retrieved aerosol optical depth at 0.55  $\mu$ m when all ABI channels used for aerosol retrieval over water are perturbed by 3% or 5% (systematic bias plus random noise).

Figure 3-4 shows the averaged uncertainty of retrieved  $\tau_{0.55\mu m}$  from tests in which TOA reflectances in all channels were perturbed by 3% and 5%. The results indicate that retrievals are within a retrieval error range of  $\pm 0.03\pm 0.05\tau$  when  $\tau_{0.55\mu m}$  is less than 1.5. AOD values larger than 1.5 are very rare over the ocean, unless dust or smoke are transported from the continents.

Since other uncertainties (e.g., estimation of surface reflectance, gas absorption correction, cloud contamination, etc.) can also lead to errors in the TOA reflectance, the above sensitivity tests could also serve as a general guide for estimating the "response" of the retrieval algorithm to these uncertainties, as well.

# 3.4.2 Physical and mathematical description for aerosol optical depth retrieval over land

# 3.4.2.1 Strategy

The ABI aerosol algorithm over land follows the similar multi-channel strategy as that over ocean. The major differences include the usage of prescribed aerosol models and estimation of surface reflection from ABI observations. This algorithm adopts the method from VIIRS with an update of accounting for the aerosol effect at the  $2.25\mu$ m channel, and adopting the land aerosol models from MODIS Collection 5 [Vermote et al., 2007; Remer et al., 2005, 2006; Levy et al., 2007].

Unlike water, land surface properties exhibit great variability and complexity, which prevent reliable modeling of the spectral reflectance. As a consequence, surface reflectance becomes an inherent unknown along with aerosol properties in the aerosol retrieval over land. Kaufman et al. [1997] observed that over vegetated and dark soil surfaces, the surface reflectance in the blue and red wavelengths correlated with the surface reflectance in the SWIR. The ABI algorithm follows the same strategy to utilize ABI channels 1, 2 and 6 (0.47, 0.64 and 2.25µm) to retrieve aerosol over dark surfaces.

Identifying dark target pixels is based on a threshold test which requires that the TOA reflectance observed in ABI channel 6 (2.25 um) is not greater than 0.25. The relationships between surface reflectances in the visible (channels 1 and 2) and in the SWIR (channel 6) are prescribed for a range of NDVIs representing various degrees of vegetation including less vegetated soil (Section 3.4.2.3). Similar to the MODIS Collection 5 algorithm, aerosol optical depth and surface reflectance are simultaneously retrieved from measurements in the blue (0.47  $\mu$ m) and SWIR (2.25  $\mu$ m) channels for each candidate aerosol models, and the optimal solution with the minimum difference between calculated and observed reflectances in the red channel (0.64  $\mu$ m) is selected.

#### 3.4.2.2 Aerosol models

Four typical aerosol models as described by Levy et al. [2007] for MODIS collection C005 are adopted in the ABI algorithm. These represent generic, dust, smoke and urban aerosols. A bimodal lognormal distribution is used to describe each aerosol size distribution:

$$\frac{dV(r)}{d\ln r} = \sum_{i=1}^{2} \frac{C_{V,i}}{\sqrt{2\pi\sigma_i}} \exp\left[-\frac{\left(\ln r - \ln r_{V,i}\right)^2}{2\sigma_i^2}\right]$$
(3.4.14)

where V(r) is the volume corresponding to particles of radii within (r, r+dr).  $C_{V,i}$  denotes

the particle volume concentration,  $I_{V,i}$  is the median radius, and  $\sigma_i$  is the associated standard deviation. Microphysical properties of the candidate aerosol models are listed below in Table 3-11. These properties are functions of the aerosol optical depth. The coefficients appearing in the functional forms that describe the dependence on optical depth are valid for finite ranges of the optical depth determined by the minimum and maximum  $(\tau_{min} \text{ and } \tau_{max})$  AOD values present in the measurements from which the coefficients are determined. Outside of this AOD range, the current ABI AOD algorithm uses values of the microphysical properties corresponding to  $\tau_{min}$  and  $\tau_{max}$ . This is in contrast to the NASA MODIS algorithm that allows the volume concentration vary with AOD even outside of the valid AOD range. This difference does have an impact on the optical properties calculated for high AOD. We also note that there is an error in Levy et al. (2007) in the representation of the imaginary part of the refractive index of the *generic* model. The sign of the coefficient representing the AOD dependence should be positive; that is, the correct complex refractive is  $1.43 - (0.008 + 0.002\tau)$ i. This is what is implemented in the NASA MODIS algorithm (Levy and Remer, private communication, March 2023). However, the reflectances in the current lookup table used in the ABI AOD algorithm were calculated with the incorrect (negative) sign.

Aerosol radiative properties are calculated with the MIE code built in the 6S RTM for spherical-particle models (generic, urban and smoke), and the Dubovik spheroid kernel software [2006] is used for dust model to account for the non-spherical shape. Precalculated aerosol radiative properties are incorporated in the radiative transfer calculation for atmospheric reflectance, transmittance and spherical albedo stored in lookup table. Note that the generic, urban, and smoke models are dominated by the fine mode, whereas the dust model is coarse-mode dominated. As the size distributions of the three fine-dominated models are similar, the main differences are in their absorption properties and refractive indices.

Aerosol Model	Mode	Volume median radius $r_V$	Stanuaru		Complex Refractive Index
Generic	Fine	$0.145+\ 0.0203 \ \tau^{\&}$	0.3738+ 0.1365 τ	$0.1642 \ \tau^{0.7747}$	1.43 - (0.008-0.002τ)i <sup>#</sup>

Table 3-11. Microphysical properties of land aerosols used in ABI algorithm

	Coarse	3.1007+ 0.3364 τ	0.7292+ 0.098 τ	$0.1482 \ \tau^{0.6846}$		
	Fine	$0.3304 \tau$ 0.1604+ 0.434 $\tau$	$0.098 \tau$ 0.3642+ $0.1529 \tau$	$0.1718 \ \tau^{0.8213}$		
Urban	Coarse	3.3252+ 0.1411 τ	0.7595+ 0.1638 τ	$0.0934 \ \tau^{0.6394}$	- 1.42 - (0.007-0.0015τ)i	
Smoke	Fine	0.1335+ 0.0096 τ	0.3834+ 0.0794 τ	$0.1748 \ \tau^{0.8914}$	1.51 - 0.02i	
Smoke	Coarse	3.4479+ 0.9489 τ	0.7433+ 0.0409 τ	$0.1043 \ \tau^{0.6824}$	1.31 - 0.021	
	Fine	$0.1416 \ \tau^{-0.0519}$	$0.7561 \ \tau^{0.148}$	$0.087 \ \tau^{1.026}$	$(1.48\tau^{-0.021}) - (0.0025$ $\tau^{0.132})i \text{ at } 0.47\mu\text{m*}$	
Dust	Coarse	2.20	0.554 τ <sup>-0.0519</sup>	0.6786 τ <sup>1.0569</sup>	$(1.48\tau^{-0.021}) - 0.002i$ at $(1.48\tau^{-0.021}) - 0.002i$ at $(1.48\tau^{-0.021}) - (0.0018\tau^{-1})^{-0.08}$ i at $0.66\mu$ m $(1.46\tau^{-0.040}) - (0.0018\tau^{-1})^{-0.30}$ i at $2.12\mu$ m	

& Aerosol optical depth ( $\tau$ ) is the spectral value at 0.55µm. The properties ( $r_v$ ,  $\sigma$  and  $C_v$ ) of smoke and generic aerosol model are defined for  $\tau$ <2.0, and  $\tau$ =2.0 is used in calculation when  $\tau$ >2.0. Likewise, parameters of urban and dust aerosol are defined for  $\tau$ <1.0, and  $\tau$ =1.0 is applied for higher  $\tau$ .

\* Refractive index at other shortwave wavelengths is estimated by spectral interpolation/extrapolation.

<sup>#</sup> It should be  $1.42 - (0.007 + 0.0015\tau)i$  (Levy and Remer, private communication, March 2023).

#### 3.4.2.3 Retrieval of land surface reflectance

Over land, contribution of the surface ( $\rho_{surf}$ ) can be comparable or even larger than the atmospheric path reflectance ( $\rho_{atm}$ ), and accuracy of aerosol retrieval for such bright surface is expected to be low. Therefore, the current algorithm retrieves aerosol only over sufficiently dark surfaces. Dark targets required by the algorithm are selected by requiring  $\rho_{2.25\mu m} \leq 0.25$ . Pixels with  $\rho_{2.25\mu m} > 0.25$  are discarded by the algorithm [Remer et al., 2005, 2006]. For the remaining dark target pixels, a set of linear relationships is used to estimate the surface reflectance at VIS channels of 0.47 and 0.64 µm from that in the SWIR 2.25-µm channel [Kaufman et al., 1997a 1997b, and 2002]. The physical reason for the spectral relationship is the simultaneous carotenoid, chlorophyll and liquid water absorption at blue, red and SWIR wavelengths associated with healthy vegetation [Kaufman and Remer, 1994].

The surface reflectance relationship is established based on collocated ABI and AERONET measurements. In version 6.1 algorithm implemented on 24 July 2018, the relationships are derived from the col-located GOES-16 ABI and AERONET data for the period of 04/29/2017 - 01/15/2018, as described in section 3.4.2.3 of ATBD version 4.2. Analysis shows that better accounting for the angular effects in surface relationship improves characterization of the ABI AOD diurnal variability. As a result, the surface reflectance relationships had another update in version 6.3 algorithm implemented on 23 October 2020 (Table A-11), where the details of the relationships are described below and are derived

from AERONET-ABI match-up data during 12/14/2017 - 12/31/2019 for GOES-16 and during 01/01/2019 - 12/31/2019 for GOES-17.

Clear sky measurements from ABI are collected at AERONET stations over the full disk domain; the criteria for selecting eligible pixels are: (1) ) separation between the pixel and station is less than 5 km horizontally and 200 meter vertically to ensure geographical adjacency, (2) average/standard deviation of AERONET aerosol optical depths within one hour centered on the ABI observation time is less than 0.6/0.2 to ensure low aerosol amount variability, (3) at least two AERONET measurements within one hour and 100 ABI observations within a circular region with a radius of 27.5 km around the site to ensure clear-sky condition, (4) AERONET Ångström Exponent (AE) calculated for 0.48 vs. 0.67µm is smaller than 0.6 or larger than 1.0 to avoid ambiguous aerosol model identification, and (5) the TOA reflectance measured in ABI channel 6 (2.25  $\mu$ m) is less than 0.25 to ensure dark surface. Atmospheric correction is performed on the selected ABI pixels with the AERONET aerosol optical depth and dust (AE < 0.6) or generic (AE > 1.0) aerosol model with the 6S-V1.1 RTM, and the retrieved surface reflectances are used as a training dataset to establish the spectral relationship between the VIS channels and the SWIR channel, namely, 0.47 vs. 2.25 µm and 0.64 vs. 2.25 µm. The offset and slope of the linear relationships are parameterized as a linear function of the solar zenith angle  $\theta_s$ , view zenith angle  $\theta_v$ , and scattering angle  $\Theta$  in degrees. The 0.47 and 0.64  $\mu$ m surface reflectances can be calculated by the formula

$$\rho_{0.47}[\rho_{0.64}] = (a_0 + a_1\theta_s + a_2\Theta + a_3\theta_v) + (b_0 + b_1\theta_s + b_2\Theta + b_3\theta_v) \times \rho_{2.25} (3.4.15)$$

where scattering angle  $\Theta$  is calculated from the corresponding relative azimuth angle  $\varphi$  as

$$\cos\Theta = -\cos\theta_s \times \cos\theta_v - \sin\theta_s \times \sin\theta_v \times \cos\varphi. \tag{3.4.16}$$

NDVI is defined as  $NDVI = \frac{\rho_{0.86}^{obs} - \rho_{0.64}^{obs}}{\rho_{0.86}^{obs} + \rho_{0.64}^{obs}}$ .

The coefficients are fitted for different NDVI ranges. They are also fitted separately for solar azimuth angle  $\leq$  or > 50° for GOES-16 (Table 3-12 and Table 3-13), and for solar zenith angle  $\leq$  or > 35° for GOES-17 (Table 3-14 and Table 3-15).

Table 3-16. GOES-16 surface reflectance relationship coefficients for solar azimuth angle  $\leq 50^{\circ}$ 

Channels (µm)	$a_0$	<i>a</i> 1	$a_2$	<i>a</i> <sub>3</sub>	$b_0$	$b_I$	$b_2$	$b_3$
				NDVI	$t \ge 0.5$			
0.47 vs. 2.25	8.934984E-04	1.597848E-04	5.802443E-05	8.153377E-05	1.320625E-01	-1.482942E-03	4.053424E-04	1.634484E-03
0.64 vs. 2.25	1.326513E-02	8.053772E-05	-2.348233E-05	-2.715831E-04	3.374356E-01	-4.894987E-04	8.045725E-04	2.232353E-03
		$0.3 \le NDVI < 0.5$						
0.47 vs. 2.25	-7.293944E-03	-2.786473E-05	1.227321E-04	4.523857E-04	2.564778E-01	-6.690913E-05	-1.548657E-04	-1.313018E-03

0.64 vs. 2.25	-4.282757E-02	-4.846731E-05	2.209718E-04	7.143245E-04	8.831485E-01	1.401954E-04	-1.461996E-03	-4.866648E-03
				$0.2 \le NL$	OVI < 0.3			
0.47 vs. 2.25	9.721227E-02	-1.167434E-03	-7.373317E-04	2.648127E-03	-3.023400E-01	4.191097E-03	4.859697E-03	-9.663053E-03
0.64 vs. 2.25	6.722176E-02	-1.202192E-03	-6.736706E-04	3.011468E-03	3.041722E-01	4.037139E-03	3.679147E-03	-1.309079E-02
				NDVI	< 0.2			
0.47 vs. 2.25	-2.770374E-02	-9.694215E-04	-4.784270E-04	4.543860E-03	4.714918E-01	3.433818E-03	2.769893E-03	-1.816880E-02
0.64 vs. 2.25	-4.540509E-02	-1.069181E-03	-5.373898E-04	5.206066E-03	7.200421E-01	5.015197E-03	3.361569E-03	-2.066685E-02

# Table 3-17. GOES-16 surface reflectance relationship coefficients for solar azimuth angle $>50^{\circ}$

Channels (µm)	<i>a</i> <sub>0</sub>	$a_1$	<i>a</i> <sub>2</sub>	<i>a</i> <sub>3</sub>	$b_0$	<i>b</i> 1	$b_2$	<i>b</i> <sub>3</sub>
(μ)				NDVI	r > 0.5			
0.47 vs. 2.25	-1.505213E-02	1.470309E-04	1.703118E-04	3.760753E-05	3.924562E-01	-7.168220E-04	-1.495472E-03	2.005906E-03
0.47 vs. 2.23	1.5052151 02	1.4705092 04				,		
0.64 vs. 2.25	1.396428E-02	-3.788400E-05	7.126271E-06	-3.716893E-04	5.638939E-01	6.803579E-04	-1.111284E-03	3.112692E-03
				$0.3 \leq NL$	OVI < 0.5	•	•	•
0.47 vs. 2.25	3.849906E-02	-8.386439E-05	-2.811522E-06	-6.778177E-05	3.739577E-02	7.223975E-04	8.356728E-05	2.290552E-03
0.64 vs. 2.25	4.339208E-02	-1.430991E-04	3.534701E-06	-4.422322E-04	2.975003E-01	1.242312E-03	-2.370100E-04	3.898779E-03
		L	L	$0.2 \le NL$	OVI < 0.3		L	•
0.47 vs. 2.25	3.085997E-02	-6.754306E-04	1.600703E-05	1.377290E-03	9.809914E-02	2.470061E-03	6.598061E-04	-3.385715E-03
0.64 vs. 2.25	2.499005E-02	-7.027014E-04	-1.572160E-04	1.876227E-03	2.484538E-01	2.348687E-03	2.697708E-03	-6.227456E-03
		NDVI < 0.2						
0.47 vs. 2.25	-5.115283E-02	1.954821E-04	-5.386475E-05	2.107060E-03	2.055075E-01	-1.672023E-03	2.911805E-03	-4.329423E-03
0.64 vs. 2.25	-3.160163E-02	3.322228E-04	-9.608414E-05	1.302774E-03	1.153388E-01	-1.643839E-03	4.284542E-03	1.748669E-03

# Table 3-18: GOES-17 surface reflectance relationship coefficients for solar zenith angle $\leq 35^\circ$

Channels (µm)	$a_0$	$a_1$	$a_2$	<i>a</i> <sub>3</sub>	$b_0$	$b_1$	$b_2$	<i>b</i> <sub>3</sub>
			•	NDVI	$\geq 0.55$		•	
0.47 vs. 2.25	1.214302E-01	-4.675449E-05	-1.407001E-04	-1.768532E-03	-9.511921E-01	-3.123009E-04	2.889237E-03	1.630940E-02
0.64 vs. 2.25	4.927811E-02	1.323502E-04	-7.836328E-05	-7.256439E-04	2.253208E-03	-9.000301E-04	2.233529E-03	5.318395E-03
		•	•	$0.35 \le NL$	OVI < 0.55	•	•	
0.47 vs. 2.25	-3.285538E-02	8.864188E-04	5.121828E-04	-6.876444E-04	3.080546E-01	-3.821264E-03	-1.580183E-03	3.794834E-03
0.64 vs. 2.25	-1.495571E-01	9.074689E-04	5.465558E-04	1.432309E-03	8.935703E-01	-2.804086E-03	-1.189015E-03	-3.720130E-03
			•	$0.26 \le NL$	OVI < 0.35	•	•	
0.47 vs. 2.25	1.189869E-01	-2.669449E-04	6.061891E-04	-2.329764E-03	-6.184802E-01	1.413153E-03	-9.738987E-04	1.391412E-02
0.64 vs. 2.25	-9.706776E-02	-3.526039E-04	6.970301E-04	1.783732E-03	5.998141E-01	4.368974E-03	-1.256832E-03	-5.012803E-03
		NDVI < 0.26						
0.47 vs. 2.25	7.023995E-02	-6.935373E-04	1.811414E-03	-4.209319E-03	2.396714E-01	4.086206E-03	-6.834570E-03	1.235253E-02
0.64 vs. 2.25	-3.839964E-01	-7.932296E-04	1.395667E-03	6.255630E-03	2.573014E+00	4.699927E-03	-4.928544E-03	-3.392500E-02

Channels (µm)	$a_0$	<i>a</i> <sub>1</sub>	$a_2$	<i>a</i> <sub>3</sub>	$b_0$	$b_1$	$b_2$	<i>b</i> <sub>3</sub>
				NDVI	$\geq 0.55$			
0.47 vs. 2.25	9.560614E-02	-2.457319E-04	-1.263887E-04	-1.225027E-03	-6.567360E-01	1.798767E-03	1.867665E-03	1.215552E-02
0.64 vs. 2.25	2.164810E-02	-2.535516E-05	-9.646596E-05	-9.476826E-05	2.226655E-01	1.221577E-03	2.060151E-03	5.142625E-04
		L	L	$0.35 \leq NL$	OVI < 0.55	L	L	L
0.47 vs. 2.25	3.714304E-03	3.780778E-04	2.996058E-04	-6.363521E-04	2.313309E-01	-1.824708E-03	-7.661543E-04	2.437708E-03
0.64 vs. 2.25	-3.847537E-02	2.862996E-04	2.553489E-04	3.345756E-04	4.381996E-01	1.207396E-04	-2.061442E-04	1.138654E-03
				$0.26 \le NL$	OVI < 0.35			
0.47 vs. 2.25	9.895028E-02	-3.026542E-04	4.058750E-04	-1.440527E-03	-3.199597E-01	1.516194E-03	-3.443628E-04	6.521642E-03
0.64 vs. 2.25	2.973293E-02	-2.660231E-04	4.120067E-04	-2.556891E-04	3.157436E-01	3.122581E-03	-2.903204E-04	-3.339985E-04
	NDVI < 0.26							
0.47 vs. 2.25	2.426597E-02	-2.735650E-04	9.734016E-04	-1.313369E-03	7.846253E-01	2.055091E-03	-3.605189E-03	-5.967014E-03
0.64 vs. 2.25	-6.216540E-02	-2.421637E-04	7.288375E-04	9.490401E-04	1.477258E+00	2.837134E-03	-2.042160E-03	-1.737660E-02

Table 3-19. GOES-17 surface reflectance relationship coefficients for solar zenith angle  $> 35^{\circ}$ 

# 3.4.2.4 Calculation of TOA reflectance

As described in Section 3.4.1.3, the TOA reflectance  $\rho_{toa}$  (Eq. 3.4.2) is the sum of atmospheric ( $\rho_{atm}$ ) and surface ( $\rho_{surf}$ ) contributions.

The atmospheric contribution, the path reflectance of the atmosphere  $\rho_{atm}$ , is modeled following Eq. 3.4.3:

$$\rho_{atm} = T^{O_3} T^{O_3} \left[ (\rho_{R+A} - \rho_R(P_0)) T^{\frac{1}{2}H_2O} + \rho_R(P) \right].$$

During the retrieval, the pre-calculated atmospheric reflectance  $\rho_{R+A}$  of a specific aerosol model and  $\tau_{550}$  is adjusted to local Rayleigh scattering and gas absorption. The look up table values are interpolated to the actual observation geometry to get the optical functions at that geometry.

Under the assumption of a Lambertian surface, the interaction between atmosphere and surface can be modeled using the adding equation of radiative transfer in a fairly simple manner [Chandrasekhar, 1960]. Therefore, the surface contribution to the TOA reflectance is calculated as:

$$\rho_{surf} = T^{O_3} T^{O_g} T^{H_2 O} \left[ T^{\downarrow}_{R+A} T^{\uparrow}_{R+A} \frac{\rho_{lam}}{1 - S_{R+A} \rho_{lam}} \right], \qquad (3.4.17)$$

where  $\rho_{lam}$  is the Lambertian land surface reflectance and the other terms are the same as in Section 3.4.1.3.

#### 3.4.2.5 Aerosol retrieval algorithm over land

Due to the relatively strong aerosol signal and low surface reflectance, TOA reflectances in the blue, red and SWIR channels are used for aerosol retrieval over land. Since three nearly independent observations allow us to extract three pieces of information, the ABI algorithm is designed to search for the appropriate aerosol model and retrieve  $\tau_{550}$  and surface reflectance by selecting the best match between ABI measurements and calculated reflectances.

The retrieval process can be described as individual retrievals for each candidate aerosol model followed by the determination of the best solution. For each aerosol model in the look-up table, the TOA reflectance in the blue and SWIR channels is used to invert  $\tau_{550}$  and the surface reflectance. The associated residual is computed as the squared difference between calculated  $\rho_{0.64}^{cal}$  and observed reflectance  $\rho_{0.64}^{obs}$  in the red channel:

$$residual = (\rho_{0.64}^{cal} - \rho_{0.64}^{obs})^2.$$
(3.4.18)

The combination of surface albedo, aerosol optical depth and aerosol model that results in the smallest, (minimum) residual is chosen as the solution.

Aerosol optical depths in five ABI channels (channels 1,2,3,5, and 6) are calculated from the spectral dependence of the aerosol normalized extinction coefficient  $n_{ext}$  of the retrieved aerosol model. Since  $n_{ext}$  for the land aerosol model is a function of  $\tau_{550}$ , the  $n_{ext,\lambda}$  is linearly interpolated to the retrieved  $\tau_{550}$ , and the optical depth at wavelength  $\lambda$  is calculated as  $\tau_{\lambda} = n_{ext,\lambda} \times \tau_{550}$ .

The procedure of simultaneous retrieval of  $\tau_{550}$  and surface reflectance is illustrated in Figure 3-5. For any given aerosol model, the retrieval is performed by looping over the aerosol optical depth  $\tau_{550}$  in the look-up table in ascending order. At any step *i* in the loop, a Lambertian surface reflectance ( $\rho_{lam,i}$ ) in the SWIR channel is retrieved based on Eq. 3.4.19, which is derived from Eq. 3.4.17:

$$\rho_{lam,i} = \frac{R}{R * S_{R+A} + T_{R+A}^{\downarrow} T_{R+A}^{\uparrow} T^{H_2 O}}$$
(3.4.19)

where  $R = \frac{\rho_{obs} - \rho_{atm}}{T^{O_3} T^{og}}$ , and  $\rho_{atm}$  is the atmospheric path reflectance corresponding to the *i*<sup>th</sup> AOD in LUT ( $\tau_{550,i}$ ). Surface reflectances at 0.47 and 0.64 µm are then estimated

through the prescribed relationships introduced in Section 3.4.2.3. When a valid  $\rho_{lam,i}$  is retrieved (value is between 0 and 1) the TOA reflectance in the 0.47-µm channel ( $\rho_{0.47,i}$ ) is calculated from  $\tau_{550,i}$  and  $\rho_{lam,i}$ . The loop of  $\tau_{550,i}$  is terminated once  $\rho_{0.47,i}$  converges to the observation ( $\rho_{0.47}^{obs}$ ). Here convergence means two adjacent steps in the loop, *i* and *i*+1, are found such that  $\rho_{0.47}^{obs}$  falls within  $\rho_{0.47,i}$  and  $\rho_{0.47,i+1}$ . The  $\tau_{550}$  for the current aerosol model is then determined by linear interpolation:

$$\tau_{550} = \tau_{550,i} * \frac{\rho_{0.47,i+1} - \rho_{0.47,i}^{obs}}{\rho_{0.47,i+1} - \rho_{0.47,i}} + \tau_{550,i+1} * \frac{\rho_{0.47}^{obs} - \rho_{0.47,i}}{\rho_{0.47,i+1} - \rho_{0.47,i}}$$
(3.4.20)

The final surface reflectance  $\rho_{lam}$  is calculated similarly from  $\rho_{lam,i}$  and  $\rho_{lam,i+1}$ .

The retrieval of 2.25-µm surface reflectance essentially finds the surface reflectance that when coupled with the atmosphere with a given aerosol optical depth results in the observed TOA reflectance  $\rho_{toa}(2.25)$ . This retrieval yields a negative surface reflectance when the atmosphere is already brighter than the observed reflectance, that is when  $\rho_{atm}(2.25) > \rho_{toa}(2.25)$  in Eq. 3.4.2. Because of the negative offsets in Eq. 3.4.15 for lessvegetated surface (low NDVI) the 0.47 and 0.64-µm surface reflectances can also become negative even when the 2.25-µm reflectance itself is positive. Negative surface albedos are unphysical and therefore must be dealt with in the retrieval. The 2.25-µm reflectance retrieval can also lead to larger than unity when the atmosphere is "too dark", that is when  $\rho_{atm}(2.25) \ll \rho_{toa}(2.25)$  even for the largest optical depth in the LUT. Since the surface is assumed Lambertian a larger than unity surface reflectance is also unphysical.

Another special case that must be treated is when the observed TOA 0.47-µm reflectance is outside of the range of the ones calculated for a given aerosol model from the aerosol optical depth values in the LUT and from the retrieved 0.47-µm surface reflectance, that is when  $\rho_{0.47}^{obs} < \rho_{0.47,1} \text{ or } \rho_{0.47,N}^{obs} > \rho_{0.47,N}$ , where N is the number of optical depth values in LUT.

Both of the above special cases are handled by extrapolation of the AOD and the surface reflectance using Eq. 3.4.20. Denoting the step by *j* in which (any of) the surface reflectance is unphysical or  $\rho_{0.47}^{obs}$  is out of range, first  $\rho_{0.47}^{obs}$  is compared to the TOA reflectance calculated for the first value of the AOD in the LUT ( $\rho_{0.47,1}$ ) and to the one calculated in step *j*-*l* ( $\rho_{0.47,j-1}$ ). If  $\rho_{0.47}^{obs}$  is closer  $\rho_{0.47,1}$  then retrievals from the first two steps ( $\tau_{550,1}, \tau_{550,2}$ ) are used in the extrapolation. Otherwise, the aerosol optical depth  $\tau_{550}$  and surface reflectance (in all channels)  $\rho_{lam}$  are extrapolated from the calculated TOA ( $\rho_{0.47,j-1}, \rho_{0.47,j}$ ) and retrieved surface reflectances ( $\rho_{lam,j-1}, \rho_{lam,j}$ ) corresponding to the optical depth values ( $\tau_{550,j-1}, \tau_{550,j}$ ) at steps *j*-*l* and *j*. The extrapolation is not performed when *j*<2; in this case no retrieval is done and all values are set to missing.

Once  $\tau_{550}$  and  $\rho_{lam}$  are determined for the current aerosol model, the residual is calculated based on Eq. 3.4.18; it is then used to select the best solution among all the candidate aerosol models after the loop over all aerosol models finished.

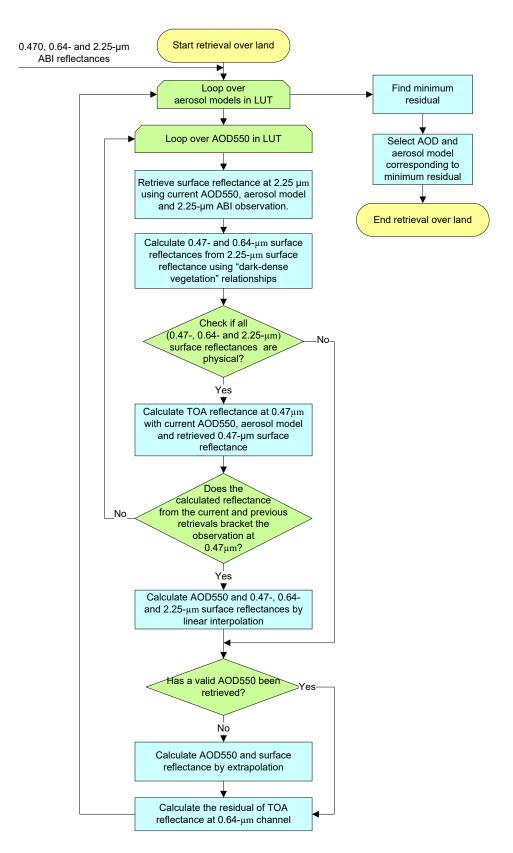


Figure 3-5. Flowchart of aerosol retrieval over land.

Compared with algorithms where transparency of aerosol in the SWIR channel is assumed, the current algorithm is expected to improve aerosol retrievals for the enhanced aerosol cases. Indeed, the pre-launch evaluation with collocated MODIS and AERONET data during the period of year 2000 to 2009 showed that the accuracy of retrieved  $\tau_{550}$  is improved by ~40% for the large AOD cases ( $\tau_{550}$ >0.8). Accounting for the aerosol effect in the SWIR channel decreases the estimated surface reflectance in that channel by ~0.003 (2.5%) and increases the retrieved  $\tau_{550}$  by ~0.012 (5.3%). Unlike the previous version of the algorithm, which assumed transparency of aerosol in the SWIR channel, the current version exhibits less preference for selecting the coarse mode aerosol model. (The previous version retrieved unrealistically large number of pixels with coarse mode aerosol.) The number of cases where dust model is selected is reduced by ~10.7%, while the number of smoke retrievals is increased by ~8.3%.

#### 3.4.2.6 Internal Tests and Quality Control

Producing a high quality global AOD product requires an effective process to screen out the contaminated pixels and identify low quality retrievals. Several simple internal tests are implemented for this purpose. Though they are not as sophisticated and particular as the dedicated algorithms, they nevertheless give the aerosol algorithm a certain degree of selfreliance and reduce the dependence on external inputs.

- 1) Internal cloud test: A brightness test,  $\rho_{0.47\,\mu m}^{obs} > 0.4$ , is used to screen out thick cloud. It should be noted that this test not only detects bright clouds, but also other bright scenes (e.g., snow and ice) unsuitable for aerosol retrievals;
- 2) Internal cirrus test:  $\rho_{1.38\mu m}^{obs} > 0.018$  is applied to avoid cirrus contamination;
- 3) Internal inhomogeneity test: In the Version 6 algorithm, standard deviation ( $\sigma_{0.47 \, \mu m}^{2\times 2}$

) is calculated from 2x2 1-km, 0.47-µm reflectances  $\rho_{0.47\mu m}^{obs}$  for each land pixel as a measure of the spatial inhomogeneity of the local retrieval area. The spatial inhomogeneity could be caused by unfavorable conditions such as sub-pixel cloud, rugged terrain, etc. The 0.47-µm channel is used due to smaller surface contribution; a land pixel will fail this test if  $\sigma_{0.47\mu m}^{2\times2} > 0.008$ . In Version 6.1 algorithm for provisional status delivery, the ABI channel reflectances at 2 km resolution are used to facilitate the implementation of the updated baseline AOD algorithm in the ground system; standard deviation ( $\sigma_{0.47\mu m}^{3\times3}$ ) is calculated from 3x3 2-km, 0.47-µm reflectances  $\rho_{0.47\mu m}^{obs}$ , and a land pixel will fail this test if  $\sigma_{0.47\mu m}^{2\times2} > 0.012$ .

- 4) <u>Internal snow test:</u> Following the MODIS algorithm, snow pixels are identified if the normalized difference snow index (NDSI) is larger than 0.3 and the brightness temperature at 11 µm is lower than 280K. Here NDSI is calculated from 0.86-µm and 1.61-µm channel reflectances as:  $NDSI = \frac{\rho_{0.86\mu m}^{obs} \rho_{1.61\mu m}^{obs}}{\rho_{0.86\mu m}^{obs} + \rho_{1.61\mu m}^{obs}};$
- 5) <u>Internal ephemeral water test:</u> Land pixels covered by ephemeral water is identified when the TOA NDVI is less than 0.1 and  $\rho_{0.86\mu m}^{obs} < 0.1$ . The latter criterion is used to ensure only dark scenes are tested. The TOA NDVI is calculated as:  $NDVI = \frac{\rho_{0.86\mu m}^{obs} - \rho_{0.64\mu m}^{obs}}{\rho_{0.86\mu m}^{obs} + \rho_{0.64\mu m}^{obs}}$ .

Based on external masks, internal tests as well as the retrieval residual, retrievals are categorized into four quality levels as listed in Table 3-20. Similar to retrievals over water, the high quality retrievals are recommended for quantitative applications due to their better overall performance; however, the lower quality retrievals can be used for qualitative examination of local episodic events due to the greater spatial coverage.

Quality Level	Criteria
No Retrieval	<ol> <li>Cloudy: input cloud mask is cloudy and any internal cloud, cirrus or inhomogeneity test fails;</li> <li>Snow/ice (from external mask or internal test);</li> <li>Ephemeral water (from internal test);</li> <li>Bright land surface (ρ<sub>2.25μm</sub> &gt; 0.25)</li> </ol>
Low	<ol> <li>Out of AOD range (-0.05, 5.0);</li> <li>Solar zenith angle &gt; 80°;</li> <li>Satellite zenith angle &gt; 60°;</li> <li>Failed internal cloud reflectance test, but external cloud mask is clear or probably clear;</li> <li>Failed internal cirrus test, but external cloud mask is clear or probably clear;</li> <li>External cloud mask is cloudy or probably cloudy, but pass internal tests, and not heavy aerosol;</li> <li>Coastal area (from external coastal mask);</li> <li>Extrapolation to positive AOD is involved;</li> <li>Retrieval residual &gt; 0.5;</li> <li>σ<sub>0.47µm</sub> &gt; 0.008 with 1-km 0.47-µm reflectances or σ<sub>0.47µm</sub></li> </ol>
Medium	<ol> <li>Adjacent to cloudy pixel;</li> <li>Adjacent to snow pixel (within 3-pixel distance);</li> </ol>

Table 3-21. Criteria used for assigning retrieval quality over land.

	3) $\sigma_{0.47\mu m}^{2\times 2} > 0.004$ with 1-km 0.47- $\mu$ m reflectances or $\sigma_{0.47\mu m}^{3\times 3} > 0.006$
	with 2-km 0.47-µm reflectances;
	4) Retrieval residual $> 0.4$ ;
	5) External cloud mask is 'probably clear';
High	Remaining retrievals

Note that after setting the quality flag to low out-of-range AOD values are re-set to the appropriate boundaries of the valid range. These truncated values are the ones that are reported in the final AOD product.

# 3.4.2.7 Sensitivity study

Tests of the sensitivity of aerosol retrieval over land to the uncertainty of TOA reflectance were performed. Similar to the tests over water, the TOA reflectances were estimated from radiative transfer calculations for the same set of geometries and aerosol optical depths. Four aerosol models used in the retrieval algorithm were adopted. Ten values of surface reflectances ranging from 0.02 to 0.2 at  $2.25\mu$ m with a constant interval of 0.02 were used. Perturbations to the ABI radiances in all channels were applied at 3% and 5% levels, which included 1) random noise; 2) positive and negative systematic biases; and 3) systematic biases plus random noise. Variation in channel-to-channel calibration was also simulated by adding a +3% bias to the individual channels. Overall, there were 13 types of perturbations with 280,000 retrieval cases for each type. Outputs from the retrievals with perturbed radiances were compared with unperturbed retrieval results to evaluate the sensitivity of the algorithm to the calibration uncertainties.

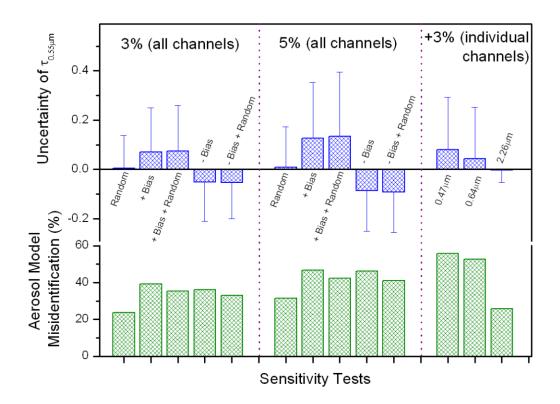


Figure 3-6. Average uncertainties in the retrieved aerosol optical depth at 0.55  $\mu$ m (top) and percentage of model misidentification (bottom) for the sensitivity tests of the aerosol retrieval over land.

The general results of the sensitivity tests are shown in Figure 3-6. The conclusions are similar to those described in Section 3.4.1.6 for the over-water retrieval. Specifically, small bias but large dispersion of retrieved  $\tau_{550}$  is associated with the random perturbation of the

TOA reflectances. The general overestimation/underestimation of  $\tau_{550}$  is associated with positive/negative biases of the TOA reflectance, with values of about 13% and 23% for the 3% and 5% systematic perturbations. This sensitivity is larger than that over water, and it can be attributed to the brighter land surface, which leads to a larger change of the TOA reflectance than that over water for the same percentage of perturbation applied. Perturbation of the individual channels also affects the retrievals with error in the 2.26-µm channel having the smallest effect. The latter is due to the fact that only small fractions of the perturbation in the SWIR channel (through the spectral relationship of surface reflection) are transferred to the uncertainty of surface reflectance and enter into the retrieval process. Model misidentification is about 35% and 40% for the 3% and 5% perturbation of reflectances. Changing the spectral shape of TOA reflectance by perturbing the radiance in a single visible channel increases the misidentification rate to more than 50%.

The large standard deviation associated with the above reported average values are due to the dependence of aerosol retrieval on geometry, surface brightness, aerosol type and loading. Examples of these dependencies are shown in Figure 3-7. It can be seen that the sensitivity of retrieved aerosol optical depth increases along with the surface reflectance, i.e., larger uncertainty is associated with brighter surface. The relative uncertainty of the retrieved  $\tau_{550}$  decreases with optical depth, while the opposite is true for the absolute uncertainty. Geometry is also an important factor; sensitivity is larger at the back and forward scattering angles. As for the dynamic model selection, due to its distinctive characteristics, identification of the dust model is the most robust; while it appears difficult to distinguish between generic and urban models at the 5% perturbation level.

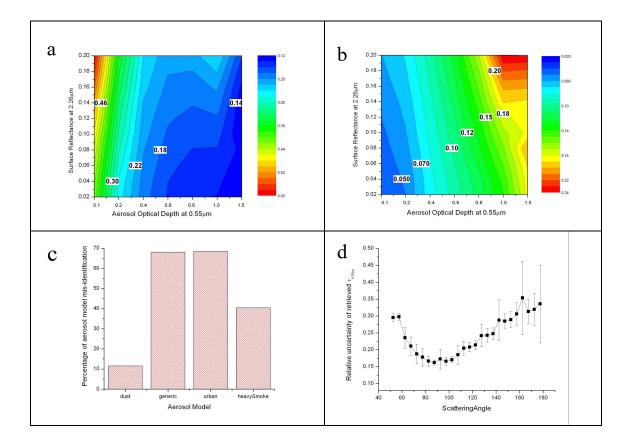


Figure 3-7. Sensitivity test results of aerosol retrieval over land with TOA reflectance increased by 5% in all channels. a) relative uncertainty of retrieved  $\tau_{550}$  as functions of surface reflectance and  $\tau_{550}$ ; b) absolute uncertainty of retrieved  $\tau_{550}$  as functions of surface reflectance and  $\tau_{550}$ ; c) percentage of misidentification for each aerosol model; d) relative uncertainty of retrieved  $\tau_{550}$  as functions of surface.

Figure 3-8 shows the averaged uncertainty of retrieved  $\tau_{550}$  as a function of AOD for the tests when all ABI channels are perturbed by 3% or 5%. It appears that, on average, the retrievals are within an error range of  $\pm 0.05 \pm 0.15\tau$  when  $\tau_{550}$  is less than 1.5.

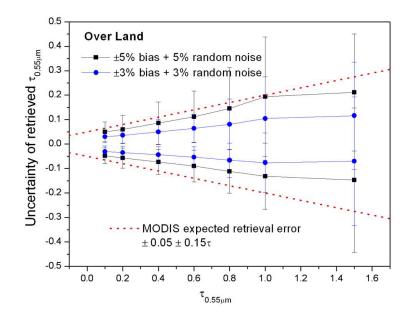


Figure 3-8.Uncertainty of retrieved aerosol optical depth at 0.55  $\mu$ m when all ABI channels used for aerosol retrieval over land are perturbed by 3% or 5% (systematic bias plus random noise).

#### 3.4.3 Calculation of aerosol size parameter

The wavelength ( $\lambda$ ) dependence of aerosol optical depth is usually described as  $\tau \propto \lambda^{-\alpha}$ , where  $\tau$  is the optical depth and  $\alpha$  is the Ångström exponent. Large/small values of the Ångström exponent indicate small/large particles, respectively. The Ångström exponent is calculated as the linear slope of aerosol optical depth versus wavelength in log scale for two wavelength pairs of (0.47, 0.86) µm and (0.86, 1.61) µm:

$$\alpha_{0.47;0.86} = -\frac{\ln \tau_{0.47} - \ln \tau_{0.86}}{\ln 0.47 - \ln 0.86}$$
(3.4.21)

$$\alpha_{0.86;1.61} = -\frac{\ln \tau_{0.86} - \ln \tau_{1.61}}{\ln 0.86 - \ln 1.61}$$
(3.4.22)

Note that the wavelength pair used to represent coarse mode particles is changed from  $(0.86, 2.25) \,\mu\text{m}$  in earlier versions to  $(0.86, 1.61) \,\mu\text{m}$ . This change is made so that AERONET ground measurements can be used in the evaluation because AERONET does

not currently have measurements at 2.25  $\mu$ m. This change also follows the practice adopted in the EPS/VIIRS algorithm.

The Ångström exponent is calculated when both optical depths at the Ångström exponent wavelength pair are positive, for example, the  $\alpha_{0.47:0.86}$  is calculated when  $\tau_{0.47} > 0$  and

 $\tau_{0.86} > 0$ .

The overall quality flag for Ångström exponent is set to 'no retrieval' when the retrieval is not applicable or fails. The quality is set to 'low' when the AOD overall quality flag (described in section 3.4.8) is 'low', or the AOD at 550nm is smaller than 0.2, or either  $\alpha_{0.47;0.86}$  or  $\alpha_{0.86;1.61}$  is out of [-1, 3] range. Otherwise it is set to 'medium'/'high' quality when the AOD overall quality flag (described in section 3.4.8) is 'medium'/'high'.

#### 3.4.4 Calculation of suspended matter mass concentration

The National Weather Service (NWS) has a requirement for PM2.5 (particulate mass in  $\mu g/m^3$  of particles smaller than 2.5  $\mu m$  in median diameter) because its models predict PM2.5 concentration. NWS therefore needs AOD to be scaled to PM2.5. This scaling would require knowledge of aerosol type and height of the aerosol layer. However, the vertical distribution of aerosols cannot be determined from ABI. Therefore, the current algorithm reports column integrated mass concentration in  $\mu g/cm^2$ .

The GOES-R ABI aerosol algorithm retrieves AOD along with one aerosol model over land and one coarse-mode and one fine-mode aerosol model with a fine-mode weight fraction over water. The retrieved AOD can be scaled into column integrated suspended matter in units of  $\mu g/cm^2$  using a mass extinction coefficient ( $cm^2/\mu g$ ) computed for the aerosol models identified by the ABI algorithm. The approach used in MODIS collection 5 was adopted [Remer et al., 2005; 2006], which converts the retrieved aerosol optical depth to column mass concentration (SM) by dividing it by the relevant mass extinction coefficient ( $B_{ext}$ ).

Over land, the mass extinction coefficients  $B_{ext}$  are function of aerosol type and AOD (Table 3-22), and the column integrated suspended matter SM is calculated as:

$$SM = \frac{\tau_{550}}{B_{ext}}.$$
 (3.4.23)

Over ocean, the final SM is obtained from combining the fine and coarse modes as:

$$SM = \frac{\tau^f}{B_{ext}^f} + \frac{\tau^c}{B_{ext}^c}, \qquad (3.4.24)$$

where  $B_{ext} = \frac{3}{4} \frac{M^{(2)}}{M^{(3)}} \frac{Q_{ext}}{d}$ ,  $Q_{ext}$  is the extinction efficiency,  $M^{(n)}$  is the n<sup>th</sup> moment of the aerosol number size distribution, (Table 3-23), and *d* is the particle density assumed to be

10<sup>6</sup> µg/cm<sup>3</sup>.  $\tau^{f} = \eta \times \tau_{550}$ ,  $\tau^{c} = (1-\eta) \times \tau_{550}$ , where  $\eta$  is the fine mode weight and  $\tau_{550}$  is the retrieved AOD at 550nm. Plug  $B_{ext}$  into Eq. (3.4.24):

$$SM = \tau_{550} \times \left[\eta \left(\frac{M^{(3)}}{\pi M^{(2)} Q_{ext}}\right)^{f} + (1 - \eta) \left(\frac{M^{(3)}}{\pi M^{(2)} Q_{ext}}\right)^{c}\right] \times \frac{4\pi d}{3} \times 10^{-12}$$
(3.4.25)

where  $\pi M^{(2)}Q_{ext}$  and  $M^{(3)}$  are the first and second quantity in Table 3-24. Since  $M^{(3)}$  is in unit of  $\mu m^3$ , a factor of  $10^{-12}$  needs to be multiplied to convert it to cm<sup>3</sup>.

In general, SM retrievals will only be validated indirectly via the comparison of ABI aerosol optical depth and particle size parameter with AERONET measurements. NWS recognizes this validation approach as adequate, as long as periodic spot check verification will also be performed/leveraged with *in situ* (aircraft) profile measurements of suspended matter. Accuracy and precision can be translated from AOD units to  $\mu g/cm^2$  units if needed but the ABI algorithm will be assessed based on AOD.

Aerosol		Aeroso	ol Model	
extinction optical	Generic	Urban	Smoke	Dust
thickness <b>7550</b>				
0.00	37.529	31.678	30.117	63.792
0.01	37.529	31.678	30.117	63.792
0.05	37.529	31.678	30.117	63.792
0.10	37.529	31.678	30.117	63.792
0.15	37.529	31.678	30.117	63.792
0.20	37.529	31.678	30.117	63.792
0.30	36.868	31.1716	29.755	64.573
0.40	35.545	30.159	29.031	66.134
0.60	33.387	28.682	27.944	68.465
0.80	31.715	27.753	27.218	70.003
1.00	30.043	26.825	26.492	71.541
1.20	29.307	26.648	26.171	72.309
1.40	28.572	26.47	25.85	73.077
1.60	27.836	26.293	25.528	73.845
1.80	27.101	26.115	25.207	74.613
2.00	26.365	25.938	24.886	75.381
2.50	26.189	25.7005	24.579	75.479
3.00	26.013	25.463	24.271	75.577
4.00	25.799	25.184	23.917	75.699

Table 3-25. Inverse of mass-extinction coefficients for over-land aerosols [cm<sup>2</sup>/µg]

<b>5.00</b> 25.584	24.905	23.563	75.822
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Table 3-26. Extinction Properties ( $\pi Q_{ext} M^{(2)}$  in cm<sup>2</sup> and  $M^{(3)}$  in  $\mu$ m<sup>3</sup>) of Ocean Aerosol Models

	Fine mode					
Model	F1	F2	F3	F4		
$\pi Q_{\rm ext} M^{(2)}$	0.9300E-10	0.2331E-09	0.5449E-09	0.1124E-08		
$M^{(3)}$	0.00070	0.00108	0.00255	0.00498		
			Coarse mode			
Model	C1 C	22	C3	C4	C5	
$\pi Q_{ext} M^{(2)}$	0.2782E-07	0.5757E-07	0.9718E-07	0.5565E-07	0.6537E-07	
$M^{(3)}$	0.31890	1.07600	2.55100	1.07600	2.10500	

# 3.4.5 Look-up table

Two lookup tables (LUT), one for the atmosphere (aerosol plus molecules at standard pressure) and one for the ocean surface reflectance, store reflectances, transmittances and other quantities pre-calculated for discrete states of the atmosphere and the ocean surface. The tables were calculated with the vector version of the 6S radiative transfer code [Vermote et al., 1997; Kotchenova et al., 2006; 2007]. The atmospheric LUT is produced for a black surface (reflectance is zero). This increases flexibility since potentially any surface can be used to couple the atmosphere with in the retrieval.

# 3.4.5.1 Atmospheric look-up table

The atmospheric LUT contains radiative functions and mass extinction coefficients used to retrieve aerosol optical depth and suspended matter mass concentration. Table 3-27 lists the contents of this LUT, the corresponding discrete values for each dimension are listed in Table 3-28.

Data Set Name	Description	Size of Dimensions
tau550	Discrete aerosol optical depth at 550nm in LUT	(20) (Ntau)
solar_zenith_angle	Discrete solar zenith angle in LUT	(21) (Nsolzen)
sensor_zenith_angle	Discrete sensor zenith angle in LUT	(25) (Nsenzen)

Table 3-29.	Contents	of the	atmospheric	look-up table

scattering_angle_position	Scattering angle indexing vector	(525) (Nsolzen x Nsenzen)
land_aer_nor_extinction_coe f	Normalized extinction coefficient for land aerosol models at ABI channel 1,2,3,5,6	(4,20,5) (NIndaer, Ntau, Nchn)
land_aer_sph_alb	Atmospheric spherical albedo corresponding to candidate land aerosol models	(4,20,3) (Nlndaer, Ntau, Nlndchn)
land_aer_trans	One-way atmospheric transmittance corresponding to candidate land aerosol models	(4,20,3,21) (Nlndaer, Ntau, Nlndchn, Nsolzen)
land_aer_refl	Atmospheric reflectance corresponding to candidate land aerosol models	(4,20,3,7727) (Nlndaer, Ntau, Nlndchn, Nscat)
water_aer_nor_extinction_co ef	Normalized extinction coefficient for ocean aerosol models at ABI channel 1,2,3,5,6	(9, 5) (Nwataer, Nchn)
water_aer_sph_alb	Atmospheric spherical albedo corresponding to candidate ocean aerosol models	(9,20,4) (Nwataer, Ntau, Nwatchn)
water_aer_trans	One-way atmospheric transmittance corresponding to candidate ocean aerosol models	(9,20,4,21) (Nwataer, Ntau, Nwatchn, Nsolzen)
water_aer_refl	Atmospheric reflectance corresponding to candidate ocean aerosol models	(9,20,4,7727) (Nwataer, Ntau, Nwatchn, Nscat)
land_aer_mass_ext_coef	Inverse of mass extinction coefficients for land aerosol models	(4,20) (NIndaer, Ntau)
water_aer_mass_ext_coef	Parameters used for computing mass extinction coefficients for ocean aerosol models	(9,2) (Nwataer,Npars)

# Table 3-30. Discrete values/description of atmospheric LUT dimensions

Dimension Name	Variable Name in Table 3-19	Number of Values	Discrete Values/Description
AOT at 550nm	Ntau	20	0.00, 0.01, 0.05, 0.10, 0.15, 0.20, 0.30, 0.40, 0.60, 0.80, 1.00, 1.20, 1.40, 1.60, 1.80, 2.00, 2.50, 3.00, 4.00, 5.00
Solar zenith angle	Nsolzen	21	0°, 4°, 8°, 12°, 16°, 20°, 24°, 28°, 32°, 36°, 40°, 44°, 48°, 52°, 56°, 60°, 64°, 68°, 72°, 76°, 80°
Sensor zenith angle	Nsenzen	25	0.0°, 2.84°, 6.52°, 10.22°, 13.93°, 17.64°, 21.35°, 25.06°, 28.77°, 32.48°, 36.19°, 39.90°, 43.61°, 47.32°, 51.03°, 54.74°, 58.46°, 62.17°,

			65.88°, 69.59°, 73.30°, 77.01°, 80.72°, 84.43°,
			88.14°
ABI channels for aerosol	Nchn	5	ABI channel 1, 2, 3, 5, 6
extinction coefficient	INCIIII	5	(0.47, 0.64, 0.865, 1.61, 2.25 μm)
ABI channels for land	Nlndchn	3	ABI channel 1, 2, 6
aerosol radiative functions	INIIdeliii	5	(0.47, 0.64, 2.25 µm)
Land aerosol models	NIndaer	4	Dust, Generic, Urban, Smoke
			Every 4° interval in the range from 180-
Soottoning on ala	Nscat	7727	$(\theta_s + \theta_v)$ to 180- $ \theta_s - \theta_v $ for all pairs combination
Scattering angle			of solar zenith angle ( $\theta_s$ ) and sensor zenith
			angle $(\theta_v)$
Ocean aerosol models	Nwataer	9	Four fine modes plus five coarse mode
ABI channels for ocean	Nwatchn	4	ABI channel 2, 3, 5, 6
aerosol radiative functions	Inwatchin	4	(0.64, 0.865, 1.61, 2.25 μm)
Parameters used for			$\beta_{ext}$ and $M^{(3)}$
computing mass	Ninora	2	extinction coefficient $[cm^2]$ and third moment
extinction coefficient for	Npars	2	of size distribution $[\mu m^3]$
ocean aerosol			

### 3.4.5.1.1 Mass extinction coefficients for land aerosols

Inverse of mass extinction coefficients are provided for four candidate land aerosol models and for each of the twenty aerosol optical depths. Linear interpolation on the optical depth dimension is needed to estimate the coefficient to convert the retrieved aerosol optical depth to the mass concentration (ATBD section 3.4.4).

### 3.4.5.1.2 Mass extinction coefficient for ocean aerosols

Two sets of parameters are provided to estimate mass extinction coefficient for the ocean aerosol models. Specifically, the extinction coefficient at  $0.55 \mu m$  ( $\beta_{ext} = \pi M^{(2)}Q_{ext}$ ) and  $M^{(3)}$  are available from LUT for each of the nine ocean aerosol models (four fine and five coarse modes), where  $M^{(n)}$  is the n<sup>th</sup> moment of the log-normal aerosol particle size distribution and  $Q_{ext}$  is the aerosol extinction efficiency. Aerosol properties and mass extinction coefficients of ocean models do not depend on the optical depth as land aerosol models do. The units of the first coefficient ( $\beta_{ext}$ ) is in cm<sup>2</sup>, and the unit of the second coefficient ( $M^{(3)}$ ) is in  $\mu m^3$ . Mass extinction coefficient is computed according to section 3.4.4 of the ATBD.

#### 3.4.5.1.3 Normalized spectral aerosol extinction coefficient

Normalized spectral aerosol extinction coefficients are provided for all the candidate aerosol models at five ABI channels (channels 1, 2, 3, 5, 6). For the land aerosol,

coefficients are available as a function of optical depth and interpolation on the optical depth dimension is needed to apply to the retrieved value.

#### 3.4.5.1.4 Spherical albedo

Atmospheric spherical albedos ( $S_{R+A}$ , subscript R+A represents combined contributions from both molecules and aerosols) are provided for each aerosol model and optical depth for channels used for retrieval. Since spherical albedo is the integrated bidirectional reflectance distribution function over both illumination and viewing hemisphere, it does not depend on geometry and there is no need for interpolation.

### **3.4.5.1.5** Transmittance

One-way atmospheric transmittances  $(T_{R+A})$  are provided for each aerosol model and optical depth for channels used for retrieval. The total transmittance is the sum of direct and diffuse components and assumed to be azimuthally invariant). Transmittances at twenty-one discrete zenith angles (for 0° to 80° in step of 4°) are provided to describe the dependence on illumination and viewing geometry. The downward and upward transmittance ( $T_{R+A}^{\downarrow}$  and  $T_{R+A}^{\uparrow}$ ) are estimated by linear interpolation of one-way transmittance LUT to the solar zenith angle and sensor zenith angle, respectively.

### 3.4.5.1.6 Reflectance

Under the plane-parallel assumption, dependence of atmospheric reflectance on geometry is usually specified by the solar zenith angle  $\theta_s$ , view zenith angle  $\theta_v$  and corresponding azimuth angles. When no provision is made for preferentially oriented scatterers, and thus scattering depends only on the angle between the incident and scattered beam (scattering angle,  $\Theta$ ), not on the incident and scattered directions separately, the dependence can be described by the scattering angle. For a given pair of  $\theta_s$  and  $\theta_v$ , the realizable scattering angle spans a range of  $[\Theta_{min}, \Theta_{max}]$  depending on the relative azimuth angle ( $\phi$ ), where  $\Theta_{min}=180^{\circ}-(\theta_s+\theta_v)$  and  $\Theta_{max}=180^{\circ}-|\theta_s-\theta_v|$ . As a result, the scattering angle range varies for different combination of  $\theta_s$  and  $\theta_v$ .

Normally, the atmospheric reflectance is calculated for discrete values of  $\theta_s$ ,  $\theta_v$  and  $\varphi$  in a lookup table to describe its angular dependence. However, such scheme leads to a varying resolution in scattering angle for different atmospheric paths. For example, there are the same number (number of discrete  $\varphi$  values) of reflectances pre-calculated for the case of  $\theta_s=10^\circ/\theta_v=10^\circ$  and the case  $\theta_s=60^\circ/\theta_v=60^\circ$ , where the former extends a range of 20° scattering angle (from 160° to 180°) and the latter spreads 120° of  $\Theta$  (from 60° to 180°). Therefore, a fixed resolution in relative azimuth angle might result in deficient or redundant representation of scattering angle dependence for certain combinations of  $\theta_s$  and  $\theta_v$ .

For the ABI aerosol retrieval algorithm, the atmospheric reflectance lookup table is generated aiming to achieve a fixed resolution (4°) in scattering angle for all the discrete combinations of  $\theta_s$  and  $\theta_v$  (there are 21 discrete values of  $\theta_s$  and 25  $\theta_v$ , a total of 525 combinations). Since the range of scattering angle varies for different ( $\theta_s$ ,  $\theta_v$ ), instead of being arranged as a rectangular array where extra space will be wasted, the reflectance entries (corresponding to a given aerosol model, aerosol optical depth, and wavelength) are organized as a one-dimensional array. Within the array, there are 525 blocks corresponding to the individual pairs of  $(\theta_s^i, \theta_v^j)$ . The sequence of blocks is ordered by looping over the viewing zenith angle first (j=1, 25) then followed by the solar zenith angle (j=1, 21). Each block contains a varying number of reflectance entries with scattering angles separated by 4° from  $\Theta_{max}$  to  $\Theta_{min}$  (the last interval might be less than 4° if  $\Theta_{max}$ -  $\Theta_{min}$  is not an integer multiple of 4°). There is a total of 7727 reflectance entries pre-calculated to represent the angular dependence of atmospheric reflectance. In order to find the block corresponding to a given  $(\theta_s^i, \theta_v^j)$ , an indexing vector with 525 elements is created to save the starting position of each block within the reflectance array. Figure 3-9 shows the layout of the atmospheric reflectance array and indexing vector and the way the starting position of each block is accessed.

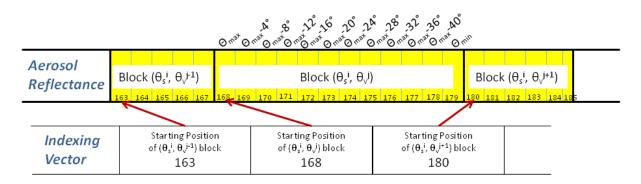


Figure 3-9. The layout of atmospheric reflectance array for a given aerosol model, aerosol optical depth and wavelength (top) and indexing vector (bottom). The starting position of each block can be accessed by the corresponding element in the indexing vector.

In the ABI aerosol retrieval, atmospheric reflectance corresponding to a given aerosol model, aerosol optical depth, wavelength and geometry ( $\theta$ s,  $\theta$ v and  $\phi$ ) is determined by linear interpolation on the values stored in the lookup table. The interpolation on geometry is implemented as follows:

- 1. The solar zenith angle bracket  $[\theta si-1, \theta si]$  containing  $\theta s$  and the linear interpolation fraction fs are determined such that  $\theta s = fs^* \theta si-1+(1-fs)^*\theta si$ .
- 2. The viewing zenith angle bracket  $[\theta v_j-1, \theta v_j]$  containing  $\theta v$  and the linear interpolation fraction fv are determined such that  $\theta v = fv^* \theta v_j-1+(1-fv)^*\theta v_j$ .
- 3. For each pair of ( $\theta$ si-1,  $\theta$ vj-1), ( $\theta$ si-1,  $\theta$ vj), ( $\theta$ si,  $\theta$ vj-1), and ( $\theta$ si,  $\theta$ vj), atmospheric reflectance corresponding to the instantaneous relative azimuth angle  $\phi$  is

interpolated from the reflectance array stored in the lookup table. For example, for the pair of ( $\theta$ si,  $\theta$ vj):

- a. The corresponding position (k) in the indexing vector is determined by k=i\*nv+j, where nv is the number of tabulated viewing zenith angle (=25), and the array index is assumed to start from zero following the convention in the C programming language. Therefore, the starting position of the block is read out from the kth element of the indexing vector, and the number of entries in this block is determined by the difference between the (k+1)th and kth elements. The block of pre-calculated reflectances corresponding to the scattering angles from Θmax to Θmin for current zenith angle pair are then extracted from the reflectance array.
- b. The scattering angle  $\Theta$  corresponding to the measurement relative azimuth angle  $\phi$  is calculated from

 $\cos\Theta = -\cos\theta \sin^2 \cos\theta v j - \sin\theta \sin^2 \sin\theta v j^* \cos\phi$ 

Linear interpolation is performed to calculate the atmospheric reflectance  $\rho_{i,j}$  of the scattering angle  $\Theta$  from the block of reflectance.

4. With the four atmospheric reflectance pi-1,j-1, pi-1,j, pi,j-1, and pi,j corresponding to the four pairs of tabulated bracket zenith angles, instantaneous atmospheric reflectance is then estimated as:

 $\rho = fs^*fv^*\rho i - 1, j - 1 + fs^*(1 - fv)^*\rho i - 1, j + (1 - fs)^*fv^*\rho i, j - 1 + (1 - fs)^*(1 - fv)^*\rho i, j$ 

# 3.4.5.2 Ocean surface reflectance look-up table

The ocean surface reflectance LUT is to account for its BRDF effect and to store the quantities needed for the analytical coupling of the atmosphere with the surface. Table 3-32 lists the contents of LUT, the corresponding discrete values for each dimension are listed in Table 3-33. There is no entry for wind direction as it is considered fixed at westerly.

Data Set Name	Description	Size of Dimensions
robar	Ocean surface diffuse reflectance $\overline{\rho_{sgt}}$ which represents the portion of downwelling atmospheric diffuse radiation reflected upward direct to the satellite sensor	(9,20,4,21,21,40,4) (Nwataer,Ntau,Nwatchn, Nsolzen,Nsenzen,Nrelazi,Nwp d)
sgalb	Ocean surface spherical albedo $\overline{\rho_{sgt}}$	(4,4) (Nwatchn, Nwpd)

Table 3-34. Contents of ocean surface reflectance look-up table

Dimension Name	Variable Name in Table 3-36	Number of Values	Discrete Values
Relative Azimuth Angle	Nrelazi	40	0°, 9°, 18°, 27°, 36°, 45°, 54°, 63°, 72°, 81°, 90°, 99°, 108°, 117°, 126°, 135°, 144°, 153°, 162°, 171°, 180°, 189°, 198°, 207°, 216°, 225°, 234°, 243°, 252°, 261°, 270°, 279°, 288°, 297°, 306°, 315°, 324°, 333°, 342°, 351°
Zenith angle	Nsolzen Nsenzen	21	0°, 4°, 8°, 12°, 16°, 20°, 24°, 28°, 32°, 36°, 40°, 44°, 48°, 52°, 56°, 60°, 64°, 68°, 72°, 76°, 80°
Wind speed (m/s)	Nwpd	4	1.0, 4.0, 6.0, 12.0

Table 3-35. Discrete values of ocean reflectance LUT dimensions

#### 3.4.5.2.1 Ocean surface reflectivity

The ocean surface sunglint diffuse reflectances  $\overline{\rho_{sgt}}$ , representing the portion of downwelling atmospheric diffuse radiation reflected upward direct to the satellite sensor, are provided for each ocean aerosol model, optical depth for the channels used in the retrieval. The dependence on geometry and surface roughness of the reflectance is represented by the extra dimensions of solar/sensor zenith angle, relative azimuth angle and wind speed. Linear interpolation on these dimensions is used to estimate the  $\overline{\rho_{sgt}}$  for any given illumination and observation geometry and surface wind speed.

With the assumption of reciprocity principle, the ocean surface diffuse reflectance  $\overline{\rho_{sgt}}$ , representing the portion of downwelling atmospheric direct radiation reflected diffusely skyward to the satellite sensor, can be regarded as  $\overline{\rho_{sgt}}$  with exchanged solar zenith ( $\theta_s$ ) and sensor zenith ( $\theta_s$ ) angles, i.e.,  $\overline{\rho_{sgt}}(\theta_s, \theta_v) = \overline{\rho_{sgt}}(\theta_v, \theta_s)$ . Consequently,  $\overline{\rho_{sgt}}$  at any given geometry and wind speed is determined via the interpolation of the  $\overline{\rho_{sgt}}$  LUT by switching the zenith angles.

#### 3.4.5.2.2 Ocean surface spherical albedo

The ocean surface sunglint spherical albedo  $(\overline{\rho_{sgt}})$  LUT is to account for the diffuse downwelling radiation that is scattered diffusely upward to satellite sensor. It is assumed to be independent of the atmosphere and therefore only a function of surface wind speed and spectral channels. There is no interpolation involved with this parameter.

# 3.4.6 Gas transmittance parameterization

To simplify the radiative transfer model in the aerosol retrieval, the transmission of gases is parameterized as an analytical function of effective absorber amount. The choice of the analytical functions was guided by the NPOESS/VIIRS aerosol algorithm. The coefficients appearing in the analytical expressions were determined for the ABI bands by applying a non-linear least squares fit to transmittances calculated by a line-by-line RTM to include continuum absorption for water vapor and ozone, and by the 6S RTM for the rest of the gases (O<sub>3</sub>, O<sub>2</sub>, CO<sub>2</sub>, N<sub>2</sub>O). In the line-by-line RTM calculation, 46 atmospheric profiles from ECWMF are utilized to cover various atmospheric conditions; while in the 6S calculation, the profiles of temperature and pressure in the standard mid-latitude summer atmosphere are used.

The analytical functions are fitted with the path absorber amount and channel-dependent coefficients C. The path absorber amount is the product of column absorber amount u and air mass M for water vapor and ozone, and it is M for other gases due to the constant content, where the column water vapor and ozone amounts are supplied as inputs to the algorithm. The air mass M is

$$M = \frac{1}{\cos(\theta_{s})} + \frac{1}{\cos(\theta_{y})}, \qquad (3.4.26)$$

where  $\theta_s$  and  $\theta_v$  are solar and local zenith angles, respectively. The fitting ranges are  $2 \le M \le 20$  for both downward and upward paths, approximating the solar and local zenith angles of  $0 \sim 85^{\circ}$ .

The transmission for water vapor is expressed as

$$T_{\lambda}^{H_2O} = \exp[C_{1,\lambda}^{H_2O} M u_{H_2O} + C_{2,\lambda}^{H_2O} \ln(M u_{H_2O}) + C_{3,\lambda}^{H_2O} M u_{H_2O} \ln(M u_{H_2O})], \quad (3.4.27)$$

where  $T_{\lambda}^{H_2O}$  is water vapor transmission at a given wavelength,  $u_{H_2O}$  is the – column water vapor amount in unit cm, and  $C_{i,\lambda}^{H_2O}$  are band-dependent coefficients. The reasonable fitting range for total precipitable water vapor is 0 ~ 40 cm. The relative fitting accuracy (fitted-calculated transmittance divided by calculated transmittance) is generally within ~1% for all channels as shown in Figure 3-10.

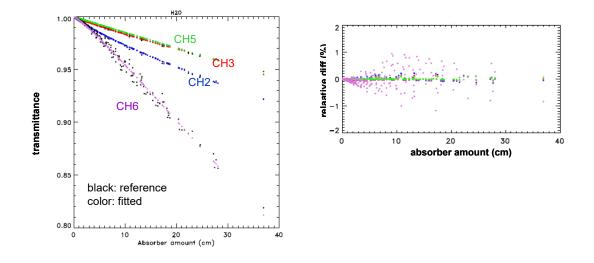


Figure 3-10. Fitting water vapor transmission (left, where original data in black and fitted data in color) and relative difference in percentage between fitted and original transmission (right) with absorber amount for ABI channels 2, 3, 5, and 6.

Similarly, ozone transmission is calculated as

$$T_{\lambda}^{O_3} = \exp(-Mu_{O_3}C_{\lambda}^{O_3}), \qquad (3.4.28),$$

where the  $u_{O_3}$  is the input column ozone amount in unit atm-cm. This function is fitted for ozone content range of  $0 \sim 600$  Dobson units. The relative fitting accuracy is again within  $\sim 1\%$ .

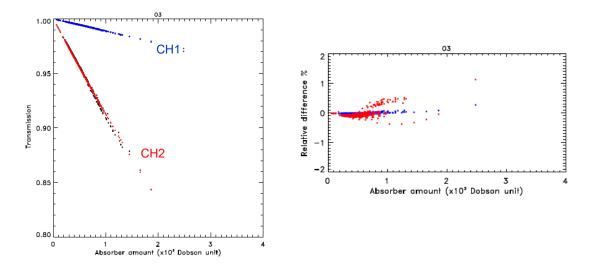


Figure 3-11. Left: Fit of ozone transmission (where original data are in black and fitted data are in color). Right: Relative difference in percentage between fitted and original transmission with absorber amount for ABI channels 1 and 2.

The transmission by gases other than water vapor and ozone, including  $O_2$ ,  $CO_2$ ,  $N_2O$ , and  $CH_4$ , is modeled as

$$T_{\lambda}^{gas_{i}} = 1.0 + C_{1,\lambda}^{gas_{i}} \times (M \times \frac{P}{P_{0}})^{C_{2,\lambda}^{gas_{i}}} , \qquad (3.4.29)$$

where  $gas_i$  represents O<sub>2</sub>, CO<sub>2</sub>, N<sub>2</sub>O, and CH<sub>4</sub> respectively, *M* is air mass, and applied with a surface pressure adjustment (ratio of actual *P* to standard surface pressure  $P_0 = 1013$  mb). The relative accuracies of fitting for other gases are well within 1%. Table 3-37 lists the fitting coefficients for corresponding ABI channels. Note that no value is provided when a specific gas does not contribute to absorption in a channel (i.e. when T=1).

The total transmittance by the other gases in Eqs. (3.4.3), (3.4.4), and (3.4.17) is calculated as:

$$T_{\lambda}^{og} = T_{\lambda}^{o_2} \times T_{\lambda}^{Co_2} \times T_{\lambda}^{N_2 O} \times T_{\lambda}^{CH_4}$$
(3.4.30)

Table 3-38.	Gas	absorp	otion	fitting	coefficients

ABI channel (wavelength in µm)	$C^{H_2O}_{1,\lambda}$	$C^{H_2O}_{2,\lambda}$	$C^{H_2O}_{3,\lambda}$	$C^{O_3}_{\lambda}$	$C^{O_2}_{1,\lambda}$	$C^{O_2}_{2,\lambda}$	$C^{CO_2}_{1,\lambda}$	$C^{CO_2}_{2,\lambda}$	$C_{1,\lambda}^{CH_4}$	$C^{CH_4}_{2,\lambda}$	$C^{N_2O}_{1,\lambda}$	$C^{N_2O}_{2,\lambda}$
1 (0.47)				0.0125								
2 (0.64)	-0.0025	-3.93e-05	0.0002	0.0853	-0.0014	0.4545						
3 (0.865)	-0.0015	-1.79e-05	6.62e-05		-1.97e-05	0.8745						
5 (1.61)	-0.0012	9.45e <b>-</b> 07	05.64e-05				-0.0221	0.6211	-0.0012	0.8549		
6 (2.25)	-0.0037	-4.03e-05	-0.0006						-0.0409	0.6883	-0.0029	0.8347

#### 3.4.7 Calculation of molecular atmospheric functions

Molecular scattering is important in the radiative transfer computation and satellite remote sensing especially in the blue spectral range. Since the blue channel is the reference (primary) channel for aerosol retrieval over land, variation of molecular reflectance and transmission need to be incorporated in an accurate and efficient manner. Instead of expanding the lookup table with an extra dimension on surface pressure, analytical formulas [Vermote and Tanré, 1992] are used in the ABI aerosol retrieval algorithm to compute molecular scattering, and to adjust the atmospheric functions pre-calculated at standard pressure to local conditions. With the contribution of polarization being implicitly considered, the analytical expressions were shown to be valid for a large range of observation conditions.

Molecular reflection is calculated as the sum of single-scattering contribution and the correction for higher orders of scatterings. The relevant formulas are from subroutine CHAND for Rayleigh scattering function in the 6S code [E. F. Vermote, D. Tanré, J. L. Deuzé, M. Herman, J. J. Morcrette, S. Y. Kotchenova, and T. Miura, Second Simulation of the Satellite Signal in the Solar Spectrum (6S), 6S User Guide Version 3 (November, 2006), <u>http://www.6s.ltdri.org</u>]. According to these the Rayleigh (molecular) reflectance  $\rho_R$  corresponding to the cosines of solar and local zenith angles,  $\mu_s$  and  $\mu_v$ , azimuth angles  $\phi_s$ ,  $\phi_v$  and Rayleigh optical depth  $\tau$  is computed as:

$$\rho_{R} = \sum_{m=0}^{2} (2 - \delta_{0,m}) \times \rho_{1}^{m}(\mu_{s}, \mu_{v}, \tau) \times \cos[(m(\pi - (\phi_{v} - \phi_{s})))] + (1 - e^{-\tau/\mu_{s}}) \times (1 - e^{-\tau/\mu_{v}}) \times \sum_{m=0}^{2} (2 - \delta_{0,m}) \times \Delta^{m}(\tau) \times P^{m}(\mu_{s}, \mu_{v}) \times \cos[(m(\pi - (\phi_{v} - \phi_{s})))]$$
(3.4.31)

Here  $\delta_{0,s}$  is the Kronecker delta,  $\rho_1^m(\mu_s, \mu_v, \tau)$  is the single-scattering reflectance corresponding to the  $m^{th}$  term of the phase function. The first three single-scattering reflectance terms (m=0, 1, 2) are:

$$\rho_1^m(\mu_s, \mu_v, \tau) = P^m \times (1 - e^{-\tau \left(\frac{1}{\mu_s} + \frac{1}{\mu_v}\right)}) \times \frac{1}{4(\mu_s + \mu_v)}$$
(3.4.32)

The first three terms of the Fourier series expansion of the Rayleigh phase function  $P^m$  (*m*=0,1,2) appearing in the equations above are:

$$P^{0} = 1 + (3\mu_{s}^{2} - 1)(3\mu_{v}^{2} - 1)*\frac{1 - \frac{\delta}{2 - \delta}}{1 + 2\frac{\delta}{2 - \delta}}*\frac{1}{8}$$

$$P^{1} = -\mu_{s}\mu_{v}(1 - \mu_{s}^{2})^{\frac{1}{2}}(1 - \mu_{v}^{2})^{\frac{1}{2}}*\frac{1 - \frac{\delta}{2 - \delta}}{1 + 2\frac{\delta}{2 - \delta}}*\beta*1.5$$

$$P^{2} = (1 - \mu_{s}^{2})(1 - \mu_{v}^{2})*\frac{1 - \frac{\delta}{2 - \delta}}{1 + 2\frac{\delta}{2 - \delta}}*\beta*0.375$$
(3.4.33)

Here  $\delta$  is the depolarization factor set to 0.0279, and the  $\beta$  factor equals to 0.5.

The Rayleigh optical depth  $\tau$  is calculated as  $\tau = \tau_0 * \frac{P}{P_0}$ , where  $\tau_0$  is the Rayleigh optical depth at standard surface pressure  $P_0$  (Table 3-39), and P is the local actual pressure.

 $\tau_0$  is pre-calculated using the 6S subroutine ODRAYL and the ABI spectral response function for standard pressure and temperature profiles.

Adjustment of optical depth  $\Delta^{s}(\tau)$  corresponding to the multiple scattering term is approximated as:

$$\Delta^m(\tau) = a^m + b^m \ln(\tau) \tag{3.4.34}$$

where m=0,1,2 and

$$\begin{aligned} a^{0} &= a_{0}^{0} + a_{1}^{0}(\mu_{s} + \mu_{v}) + a_{2}^{0}\mu_{s}\mu_{v} + a_{3}^{0}(\mu_{s}^{2} + \mu_{v}^{2}) + a_{4}^{0}(\mu_{s}\mu_{v})^{2}, \\ \left\{a_{n}^{0}\right\}_{n=0,1,\dots,4} &= \{\ 0.332438,\ 0.162854,\ -0.309248,\ -0.103244,\ 0.114933 \ \} \text{ and} \\ b^{0} &= b_{0}^{0} + b_{1}^{0}(\mu_{s} + \mu_{v}) + b_{2}^{0}\mu_{s}\mu_{v} + b_{3}^{0}(\mu_{s}^{2} + \mu_{v}^{2}) + b_{4}^{0}(\mu_{s}\mu_{v})^{2}, \\ \left\{b_{n}^{0}\right\}_{n=0,1,\dots,4} &= \{\ -6.7771(10^{-2}),\ 1.577(10^{-3}),\ -1.2409(10^{-2}),\ 3.2417(10^{-2}),\ -3.5037(10^{-2})\}. \\ \text{and} \ a^{1} &= 0.19666,\ a^{2} &= 0.145459 \ ;\ b^{1} &= -0.054391,\ b^{2} &= -0.029108 \ . \end{aligned}$$

Table 3-40. Rayleigh optical depth at standard surface pressure for ABI channels

ABI Channel (wavelength: μm)	$ au_0$
1 (0.47)	0.1852
2 (0.64)	0.0542
3 (0.86)	0.0157
5 (1.61)	0.0013
6 (2.25)	0.0003

Rayleigh reflectance  $\rho_R$  is calculated at actual surface pressure and standard pressure, respectively, and used in Eq. (3.4.3) in Section 3.4.1.3. The dependence on pressure is realized through the Rayleigh optical depth  $\tau$  that enters in the calculation of the Rayleigh reflectance.

The Rayleigh transmission  $T_R(\mu)$  and spherical albedo  $S_R$  are used to correct the optical functions stored in LUT to the local pressure, which are computed at standard surface pressure. Specifically, the LUT transmissions  $T_{R+A}^{\downarrow}$  and  $T_{R+A}^{\uparrow}$  in Eq. (3.4.4) and in Eq. (3.4.17) need to be multiplied by the ratio of Rayleigh transmission  $T_R(\mu)$  at actual pressure to that at standard pressure; the LUT spherical albedo  $S_{R+A}$  in Eq. (3.4.4) and in Eq.(3.4.17) is corrected by adding the difference between the Rayleigh spherical albedo  $S_R$  at actual pressure and that at standard pressure. The pressure correction is realized through the Rayleigh optical depth  $\tau$ .

The analytical expression of Rayleigh transmission function is based on the two-stream method,

$$T_{R}(\mu) = \frac{\left[\frac{2}{3} + \mu\right] + \left[\frac{2}{3} - \mu\right]e^{-\tau/\mu}}{\frac{4}{3} + \tau}$$
(3.4.35)

where  $\mu$  is the cosine of the solar / view zenith angle for downward/upward transmittance, respectively.

For conservative molecular scattering, the spherical albedo S is given by:

$$S_{R} = \frac{1}{4+3\tau} [3\tau - 4E_{3}(\tau) + 6E_{4}(\tau)]$$
(3.4.36)

where  $E_n$  is the exponential integral ( $E_n(x) = \int_1^\infty \frac{e^{-xt}}{t^n} dt$ ). The exponential integral is estimated as:

$$E_1(\tau) = \sum_{i=0}^5 c_i \tau^i - \ln \tau , \qquad (3.4.37)$$

Where  $\tau$  is the Rayleigh optical depth, coefficients  $c_i = -0.57721566$ , 0.99999193, -0.24991055, 0.5519968, -0.00976004, 0.00107857 for *i*=0 to 5. The recurrence relation is used to calculate  $E_n(x)$  for n>0:

$$E_{n+1}(\tau) = \frac{1}{n} (e^{-\tau} - \tau E_n(\tau)).$$
(3.4.38)

#### 3.4.8 Algorithm output

The final output of this algorithm includes aerosol optical depth, aerosol type, particle size parameter, and suspended matter mass concentration. Aerosol type is an intermediate product used mainly in detailed analysis of the AOD retrieval, but it also used by the GOES-R Shortwave Radiation Budget (SRB) algorithm. The parameters are given below in Table 3-25. The overall quality flag is set to 'no retrieval' when the retrieval is not applicable or fails, and set to 'low', 'medium' or 'high' quality from the quality control process.

<u>Important caveat</u>: Table 3-42 lists the parameters in the output file from the GOES-R AOD science code. The output file generated in the GOES-R Ground Segment (GS) and distributed to users, however, does not include all parameters listed in Table 3-43. The parameters not in the GS output file include detailed quality flags and identification of source of all inputs, internal test flags, critical path flags, particle size, suspended matter mass concentration, etc. Users of the GS output files should consult Volume 5 of the PUG (Level 2+ products) to see the content of those files.

Table 3-44 . ABI aerosol	algorithm	output
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Name	Туре	Description	Dimension
AOD at 550nm	output	Retrieved aerosol optical depth at 550 nm	Grid (xsize, ysize)
AOD in ABI channels	output	Retrieved aerosol optical depth in ABI channels 1,2,3,5,6	Grid (xsize, ysize) x 5
Particle size	output	Ångström Exponents (proxy for particle size) calculated from AOD at two pairs of wavelengths (0.47,0.86 µm and 0.86,1.61 µm)	Grid (xsize, ysize) x 2
Suspended matter mass concentration	output	Column aerosol mass	Grid (xsize, ysize)
Overall QC flag	output	Overall quality flag for aerosol retrieval: 3: no retrieval 2: low quality 1: medium quality 0: high quality	Grid (xsize, ysize)
Detailed QC flags	output	Detailed input and output quality and critical path flags (see Table 3-45)	Grid (xsize, ysize)
Aerosol type ID	intermediate	Aerosol model selected from prescribed models during the retrieval; 0: oceanic aerosol; 1: dust over land; 2: generic aerosol over land; 3: urban aerosol over land; 4: smoke over land.	Grid (xsize, ysize)
Fine mode aerosol index	diagnostic	Index of fine mode aerosol model over ocean	Grid (xsize, ysize)
Coarse mode aerosol index	diagnostic	Index of coarse mode aerosol model over ocean	Grid (xsize, ysize)
Fine mode weight	diagnostic	Fine mode weight over ocean	Grid (xsize, ysize)
Land surface reflectance	diagnostic	Surface reflectance of land retrieved in three channels (1,2 and 6)	Grid (xsize, ysize) x 3
Residual	diagnostic	Retrieval residual of best solution	pixel (xsize, ysize)
Homogeneity standard deviation	diagnostic	Standard deviation of TOA reflectance at Ch1/Ch61 (land/ocean)	pixel (xsize, ysize)

Byte	Bits	Quality Flag Name	Meaning
1: Input Geometry Quality Flag: QCInputGeo	0	QC_INPUT_LON	0: valid longitude (-180 - 180°) 1: out-of-range longitude
	1	QC_INPUT_LAT	0: valid latitude (-90 - 90°) 1: out-of-range latitude
	2	QC_INPUT_ELEV	0: valid elevation (-2000 – 10,000 m) 1: out-of-range elevation
	3	QC_INPUT_SOLZEN	0: valid solar zenith (0 - 90°) 1: out-of-range solar zenith
	4	QC_INPUT_SATZEN	0: valid satellite zenith (0 - 90°) 1: out-of-range satellite zenith
	5	QC_INPUT_SOLAZI	0: valid solar azimuth (-180 - 180°) 1: out-of-range solar azimuth
	6	QC_INPUT_SATAZI	0: valid satellite azimuth (-180 - 180°) 1: out-of-range satellite azimuth
	0	QC_INPUT_TPW_ABI	0: TPW data from ABI retrieval 1: TPW data not from ABI retrieval
	1	QC_INPUT_TPW_MODEL	0: TPW data from model 1: TPW data not from model
	2	QC_INPUT_OZONE_ABI	0: ozone data from ABI retrieval 1: ozone data not from ABI retrieval
2: Input	3	QC_INPUT_OZONE_MODEL	0: ozone data from model 1: ozone data not from model
Ancillary Data Flag: QCInputAnc	4	QC_INPUTPRES	0: valid model surface pressure (500 – 1500 mb) 1: constant surface pressure (1013 mb)
<b>C F</b>	5	QC_INPUT_HGT	0: valid model surface height (-2 – 10 km) 1: constant surface height (0 km)
	6	QC_INPUT_WSP	0: valid model surface wind speed (0 – 100 m/s) 1: constant surface wind speed (6 m/s)
	7	QC_INPUT_WDR	0: model surface wind direction (0° - 360°) 1: fixed surface wind direction (90°)
3: Input Reflectance Data Flag: QCInputRef	0	QC_INPUT_REFL_CH1	0: valid ABI reflectance in band 1 (0 – 1) 1: out-of-range ABI reflectance in band 1
	1	QC_INPUT_REFL_CH2	0: valid ABI reflectance in band 2 (0 – 1) 1: out-of-range ABI reflectance in band 2
	2	QC_INPUT_REFL_CH3	0: valid ABI reflectance in band 3 (0 – 1) 1: out-of-range ABI reflectance in band 3
	3	QC_INPUT_REFL_CH4	0: valid ABI reflectance in band 4 (0 – 1) 1: out-of-range ABI reflectance in band 4

 Table 3-46 Detailed input and output quality and critical path flags

1	-		
	4	QC_INPUT_REFL_CH5	0: valid ABI reflectance in band 5 $(0-1)$ 1: out-of-range ABI reflectance in band 5
	5	QC_INPUT_REFL_CH6	0: valid ABI reflectance in band 6 $(0 - 1)$ 1: out-of-range ABI reflectance in band 6
	6	QC_INPUT_BT11	0: valid ABI brightness temperature in band 14 (200 – 350 K) 1: out-of-range ABI brightness temperature in band 14
4: Internal Test Flag: QCTest	0	QC_CLOUDY	0: no cloud by internal reflectance check 1: cloud by internal reflectance check
	1	QC_CIRRUS	0: no cirrus by internal check 1: cirrus by internal check
	2	QC_INHOMO	0: homogeneity by internal check 1: inhomogeneity by internal check
	3	QC_SNOWICE	0: no snow/ice by internal check 1: snow/ice by internal check
	4	QC_EPHEMERAL_WATER	0: no ephemeral water by internal check 1: ephemeral water by internal check
	5	QC_SHALLOW_WATER	0: no shallow water by internal check 1: shallow water by internal check
	6	QC_WATER_GLINT	0: no sunglint by internal check 1: sunglint by internal check
	7	QC_LAND_BRISFC	0: dark surface 1: bright surface
5: Critical Path Flag: QCPath	0	QC_CLOUD_MASK	0: clear sky by cloud mask 1: cloudy sky by cloud mask
	1	QC_RET_SCENE	0: over-land algorithm is used 1: over-water algorithm is used
	2	QC_LAND_TYPE	0: vegetation 1: soil
	3	QC_SNOW	0: no snow/ice by snow mask 1: snow/ice by snow mask
	4	QC_COAST	0: not coast area by mask 1: coast area by mask
	5	QC_SHALLOW_LAND_WATE R	0: not shallow inland water by mask 1: shallow inland water by mask
	6	QC_SHALLOW_OCEAN	0: not shallow ocean by mask 1: shallow ocean by mask
	7	QC_HEAVY_AEROSOL	0: not heavy aerosol by mask 1: heavy aerosol by mask
	0	QC_AOD	0: AOD is retrieved 1: AOD is not retrieved

6: AOD Product Quality Flag: QCAOD	1	QC_RET_EXTRP	0: interpolation within LUT AOD range 1: extrapolation of AOD used
	2	QC_OUT_SPEC	0: within F&PS specification range 1: out of F&PS specification range
	3	QC_LOWSUN	0: solar zenith angle not larger than 80° 1: solar zenith angle larger than 80°
	4	QC_LOWSAT	0: local zenith angle not larger than 60° 1: local zenith angle larger than 60°
	5	QC_ADJ	0: not adjacent to cloud or snow 1: adjacent to cloud or snow

In addition, the following metadata information is included in the output:

- DateTime (swath beginning and swath end)
- Bounding Box
  - product resolution (nominal and/or at nadir)
  - o number of rows and
  - o number of columns,
  - o bytes per pixel
  - o data type
  - $\circ$  byte order information
  - location of box relative to nadir (pixel space)
- Product Name
- Product Units
- Ancillary Data to Produce Product (including product precedence and interval between datasets is applicable)
  - Version Number
  - Origin (where it was produced)
  - o Name
- Satellite
- Instrument
- Altitude
- Nadir pixel in the fixed grid
- Attitude
- Latitude
- Longitude
- Grid Projection
- Type of Scan
- Product Version Number
- Data compression type
- Location of production
- Citations to Documents
- Contact Information

- Mean and standard deviation of AOD retrievals at 550nm and ABI channels 1, 2, 3, 5, 6 over land
- Mean and standard deviation of AOD retrievals at 550nm and ABI channels 1, 2, 3, 5, 6 over ocean
- Maximum and minimum AOD retrievals at 550nm and ABI channels 1, 2, 3, 5, 6 over land
- Maximum and minimum AOD retrievals at 550nm and ABI channels 1, 2, 3, 5, 6 over ocean
- For each QA flag value, the following information is required:
  - Percent of retrievals with the QA flag value
  - Definition of QA flag
- Total number of pixels where retrieval was attempted separately for land and ocean
- Number of pixels with local zenith angle less than 60 degrees
- For each 10° latitude zone and surface type:
  - Zonal min, max, mean and standard deviation of AOD at 550nm over land and ocean, respectively
  - Zonal min, max, mean and standard deviation of AOD at ABI channels 1, 2, 3, 5, 6 over land and ocean, respectively
  - Zonal min, max, mean and standard deviation of surface reflectivity at ABI channel 1, 2 and 6 over land
  - Geographic bounding box
  - For each QA flag value, the following information is required:
    - Percent of retrievals with the QA flag value
    - Definition of QA flag
  - Total number of pixels where retrieval was attempted separately for land and ocean
  - Number of pixels with local zenith angle less than 60 degrees

# **4 TEST DATA SETS AND OUTPUTS**

# 4.1 Input Data Sets

Proxy clear-sky TOA reflectances in the ABI bands were used for algorithm development and testing. Such data can be obtained from observations of existing satellites. For example, MODIS reflectances could be used because the spectral placement of the MODIS channels is similar to those of ABI (Table 4.1). The advantage of this approach is that the scenes are realistic. However, some of the MODIS channels do not exactly match the ABI channels so appropriate spectral transformations would be needed to convert the MODIS reflectances to ABI reflectances. Such conversions can only be derived from radiative transfer calculations for different (but a limited number of) atmospheric and surface conditions (scenes). These transformations are not expected to hold for all possible scenes encountered in real observations. One can avoid the spectral conversion if the banddependent components of the algorithm (e.g. LUT) are built for the MODIS band. In this case, however, one is not fully testing the ABI algorithm. Another possibility for generating proxy reflectances is to simulate them with a radiative transfer model. The advantage is that one can "match" the ABI channels exactly, and the "true" AOD is also known. However, this approach can only offer a limited realism and because of its nature must be confined to specific, very limited scenes. A third possibility, which was adopted for the ABI aerosol algorithm development, combines the best of the two approaches mentioned above. In this method, MODIS derived atmospheric (cloud mask, AOD, total column ozone and water vapor) and surface (8-day composite surface reflectance) properties are used with solutions of radiative transfer calculation represented in the form of LUT as described in the next section [Laszlo et al., 2007].

ABI Channel	MODIS Channel
Channel 1: 0.47µm	Channel 3: 0.47µm
Channel 2: 0.64µm	Channel 1: 0.66µm
Channel 3: 0.86µm	Channel 2: 0.86µm
Channel 4: 1.38µm	Channel 26: 1.38µm
Channel 5: 1.61µm	Channel 6: 1.64µm
Channel 6: 2.26µm	Channel 7: 2.13µm

Table 4-1. Channel mapping between ABI and MODIS

# 4.1.1 Development of a fast simulator to simulate cloud-free ABI TOA reflectance

To simulate cloud-free radiance fields in six ABI bands, i.e., 0.47, 0.64, 0.865, 1.378, 1.61 and 2.25 µm, a fast ABI simulator was developed. This scheme bypasses time-consuming RT calculations by using pre-calculated look-up tables and empirical relationships. Inputs required for the simulations, including bidirectional reflectance distribution function (BRDF) of land surface, aerosol optical depth and type, total amount of ozone and water vapor, are obtained from MODIS products. The advantage of this scheme lies in three aspects. First, it is designed to substantially reduce CPU time; for example, the computational time for one MODIS granule is reduced from about two weeks with direct 6S RT simulation to less than 10 minutes with the LUT with nearly 80% coverage of aerosol retrievals. Second, the speed of the fast scheme is not achieved at the cost of the accuracy, as the difference in TOA reflectance between the fast scheme and 6S RTM calculation is less than 3%. Third, the fast scheme applies to both land and ocean. In brief, the fast scheme is able to efficiently generate TOA radiance fields for developing and validating the aerosol retrieval algorithm, not only for an individual granule, but also for global coverage with sufficient accuracy. The flowchart of the fast simulator is shown in Figure 4-1.

#### 4.1.1.1 One MODIS/Terra granule for dust case over ocean

As an example, reflectances simulated for four ABI channels (2, 3, 4 and 6) for one MODIS/Terra granule on September 30, 2002 over ocean are presented in Figure 4-2. The

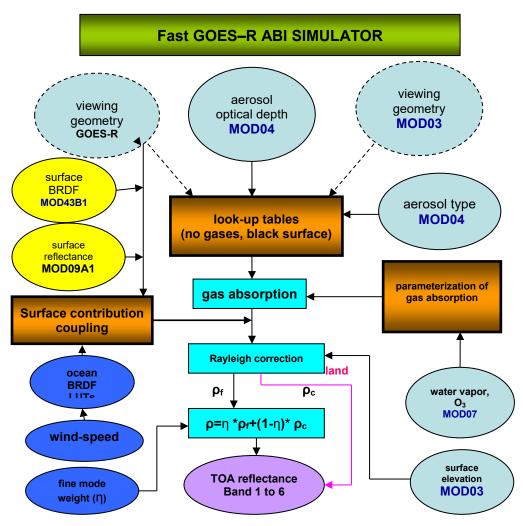


Figure 4-1. Flow chart of fast simulation scheme for GOES-R ABI radiance field.

RGB image for this granule is also shown. This scene has scattered clouds mixed with small aerosol loading (AOD <0.5). This is also shown in the MODIS retrieved aerosol optical depth at 550 nm (top right in Figure 4-2), which is one of the inputs to the simulation scheme. The fine mode weight (another input) indicates that aerosols in this scene are dominated by fine mode. The map of wind speed shows that most parts of the scene have moderate roughness; however, high wind (up to 14 m/s) is seen in the upper-left corner of the granule and at the middle of the left edge, where slightly higher fine mode aerosol loading appears. Note that the black patch in the center of the simulated reflectance fields is the place where the sunglint angle is less than 40 and no retrieval was performed by the MODIS aerosol algorithm.

### 4.1.1.2 Two MODIS/Aqua granules for smoke case over land

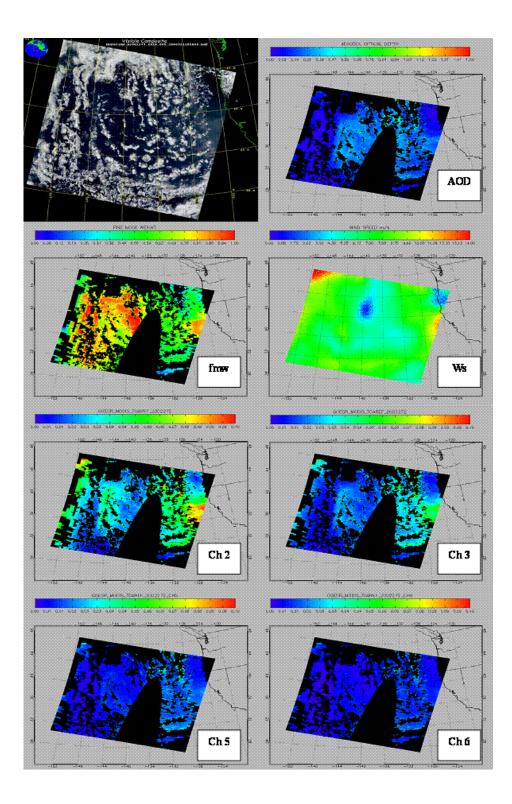
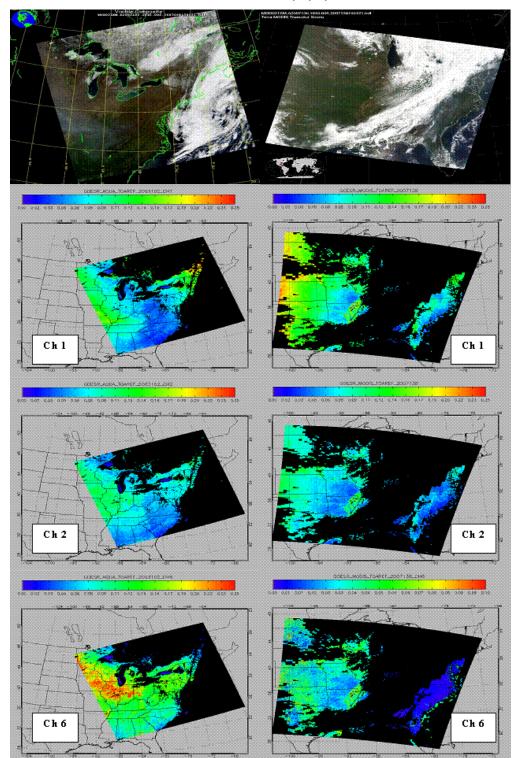


Figure 4-2. Example of ABI reflectances simulated from one MODIS/TERRA granule at UTC 20:10 on September 30 (day 273), 2002. Top left: RGB image; top right: AOD: aerosol optical depth at 550 nm; second row left: fine mode to



coarse mode optical depth weight (FMW); second row right: wind speed; third and fourth rows: simulated for channel 2, 3, 5, and 6 reflectances.

Figure 4-3. Reflectance fields simulated for MODIS/AQUA granules at UTC: 18:15 on April 12, 2003 (left panel) and at UTC 16:45 on May 16, 2007 (right panel). RGB images are shown in the top row.

Figure 4-3 shows simulations for two MODIS granules over land. One is from April 12, 2003 and the other is from May 16, 2007. Both cases contain smoke from wild fires. These can be seen in the RGB images. For the case on April 12, 2003, higher surface reflectance is indicated in TOA reflectance in Channel 6 as a result of lower vegetation coverage.

### 4.1.2 MODIS radiance as proxy data sets

In addition to proxy data from the fast simulator, clear-sky MODIS reflectances are also used as proxy data for algorithm development and evaluation. This is because the MODIS channels have spectral placement and width similar to those of ABI. For this, new LUTs specific to the MODIS channels and band passes were created using the 6S radiative transfer model. Cloud screening, dark land surface selection and quality assurance are performed following the MODIS scheme. Hereafter the ABI algorithm with direct inputs of MODIS products is referred to as the ABI/MODIS algorithm.

The ground-based remote sensing network, AEROsol Robotic Network (AERONET), equipped with well-calibrated sunphotometers over more than 100 sites throughout the world, measures and derives quality-assured aerosol optical properties for a wide diversity of aerosol regimes, for up to the last 10 years [Holben et al., 1998; 2001; Dubovik et al., 2002]. These high-quality data have been widely used as ground "truth" for evaluation and validation of satellite remote sensing of aerosols [Yu et al., 2003; Remer et al., 2005].

AERONET version 2 level 2.0 data and MODIS collection 5 aerosol product for the years 2000-2009 (2000-2009 for Terra and 2002-2008 for Aqua) are collected, collocated and analyzed. The collocation follows the MODIS validation strategy [Ichoku et al., 2002; Remer et al., 2005], in which AERONET data is temporally averaged within a one-hour window around the MODIS overpass time and the MODIS data are spatially averaged in a 50x50 km box centered on the AERONET station. The MODIS reflectances used here are the gas-absorption corrected reflectances available in the MODIS aerosol product. Because of this, this procedure does not test calculation of the gas absorption implemented in the ABI aerosol algorithm.

# 4.2 Output Analysis from Input Data Sets

## 4.2.1 **Precisions and accuracy estimates**

The validation of the aerosol products compares satellite-retrieved AOD and ASP with reference ("truth") values, and it involves calculation of certain metrics that characterize the level of agreement between the satellite retrievals and reference values. The reference

data include (1) aerosol data used in the simulation of ABI radiances, and (2) measurements of aerosol properties made from the ground measurements. The primary means of validation is the comparison with the ground measurements made at the AERONET sites. Evaluation is also done by performing retrievals from model-simulated proxy ABI data, and by comparing the retrieved aerosol product to the known aerosol input used in the forward simulation. This type of validation is ideal for "deep-dive" evaluation of the algorithm because all relevant data are known from the simulations. It is, however, necessarily limited to scenes selected for simulation.

Performance of the ABI aerosol algorithm is measured by two metrics: precision and accuracy of the retrievals. AWG defines

- Accuracy as the mean difference (bias, systematic error) between the retrieved and reference "truth" values. The ABI retrievals and reference data should be appropriately averaged in space and time to avoid sampling issues.
- Precision is defined as the standard deviation of the differences between ABI and reference data representing the random error of ABI products.

In addition to the accuracy and precision other commonly used statistics, like the root mean square error (RMSE) of the differences and correlation between ABI and reference data, are also calculated. Histograms of the differences are also analyzed. The ABI aerosol products are considered validated if the overall accuracy and precision satisfy the requirements specified in the F&PS and MRD.

## 4.2.1.1 Estimates using simulated input radiances

The ABI algorithm was tested with TOA reflectances simulated using the fast simulator described in Section 4.1.1. Figure 4-4 shows the comparison of ABI AOD and fine-mode weight (FMW) retrieved over ocean with reference values obtained from a MODIS granule over the North Pacific Ocean near the North American Continent on day 273 of 2002. A good agreement is seen with correlation coefficients 0.99 for both AOD and FW. The mean differences are 0.00017 and 0.00069, and standard deviations are 0.00043 and 0.00354 for AOD and FW, respectively. The analysis shows that the relatively large differences between the MODIS reference and ABI-retrieved FWs are associated either with relatively small optical depth (AOD  $\leq$  0.1) or with relatively large AOD retrieval error (ABI retrieval –MODIS input AOD > 0.02).

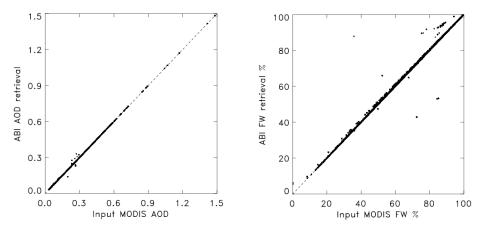


Figure 4-4. Comparison of AOD (left) and fine-mode weight (FW) in percentage (right) from the MODIS reference with those retrieved from the ABI algorithm for a selected test scene over ocean.

Figure 4-5 shows an example of validating AOD retrieved over land with MODIS input AOD used in the simulation for two days. As seen for May 16, 2007, the agreement is relatively good; the mean difference is only 0.0005 ( $\sim 0.2\%$  difference) and the standard deviation is 0.0006. However, for day April 12, 2002, the mean difference and RMS can be as large as 0.02 and 0.023 ( $\sim 11\%$  difference), respectively.

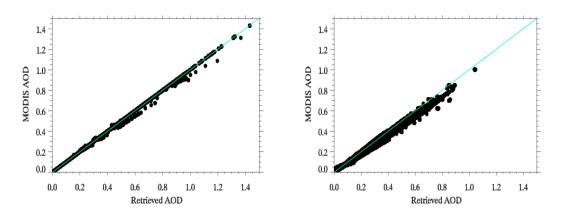


Figure 4-5. Comparison of retrieved and reference (MODIS) AOD for two MODIS granules: (left) May 16, 2007, (right) April 12, 2002.

### 4.2.1.2 Estimates using MODIS reflectances

An extensive collocated MODIS-AERONET dataset for the years 2000-20012 are used for the retrieval of aerosol with the ABI algorithm and for the evaluation of the retrieved product. The gas-absorption-corrected "aerosol" reflectances in the MODIS aerosol product are used as proxy inputs to the ABI/MODIS aerosol algorithm. For the comparison with the ground measurements, the AERONET data at 550 nm are linearity interpolated between the 440- and 870-nm AOD values in log-log space. Note that the range of AOD reported in ABI, MODIS and AERONET are different. The ABI retrievals have a product measurement range for AOD of [-1.0, 5.0]. MODIS reports negative values up to -0.05, but over land only; it does not report negative values over water. AERONET do not allow negative values. Therefore, the total number of samples used in the comparisons of ABI with reference data depends on whether the reference data are the MODIS retrievals or the AERONET values.

Table 4-2 and Table 4-3 show the overall statistics between ABI/MODIS AODs with AERONET measurements at 550 nm. Generally, ABI and MODIS statistics are comparable over land; the ABI bias is somewhat smaller over ocean, most likely due to using variable wind speed in the calculation of surface reflectance of water. Figure 4-6 and Table 4-4 show the accuracy and precision values for the different AOD ranges specified in the F&PS. The results indicate the AOD product meets the 100% F&PS requirements.

Table 4-2. AOD validation statistics over land obtained from the collocated AERONET-MODIS dataset for years 2000-2012. RMSE is the root mean square error. MinErr and MaxErr are minimum and maximum differences, respectively.

	Accuracy	Precision	RMSE	Correlation	MinErr	MaxErr
ABI	0.028	0.140	0.143	81.6%	-2.205	2.428
MODIS	0.027	0.122	0.125	86.7%	-1.887	3.331

Table 4-3. AOD validation statistics over ocean obtained from the collocated AERONET-MODIS dataset for years 2000-2012. RMSE is the root mean square error. MinErr and MaxErr are minimum and maximum differences, respectively.

	Accuracy	Precision	RMSE	Correlation	MinErr	MaxErr
ABI	0.013	0.078	0.079	88.6%	-1.013	2.546
MODIS	0.018	0.082	0.084	88.0%	-0.976	2.540

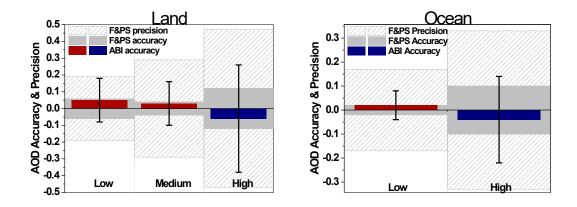


Figure 4-6. Comparison of ABI AOD with AERONET AOD at 550 nm over land (left) and over ocean (right) using collocated AERONET-MODIS dataset for years 2000-2012.

Table 4-4. Accuracy and precision of ABI AOD from comparison with AERONET AOD at 550 nm over land (left) and over water (right) using collocated AERONET-MODIS dataset for years 2000-2012. F&PS requirements are in parenthesis.

Land					Ocean			
Range	AOD	Accuracy	Precision	# of points	AOD	Accuracy	Precision	# of points
Low	< 0.04	0.05 (0.06)	0.13 (0.13)	25,581	-0.4	0.02	0.06	40.260
Medium	0.04 - 0.8	0.03 (0.04)	0.13 (0.25)	162,252	62,252 <0.4	(0.02)	(0.15)	40,269
High	> 0.8	-0.06 (0.12)	0.32 (0.35)	4,295	>0.4	-0.04 (0.10)	0.18 (0.23)	3,316

Figure 4-7 displays the histogram of the Ångström Exponent (AE) derived from ABI, MODIS and AERONET. The distribution of ABI and MODIS AE are similar. Both show two peaks (~0.6 and ~1.7) over land. These peaks correspond to the assumed fine and coarse modes. The AERONET AE also peaks around 1.4 but it does not have a peak at the small AE. In contrast, over water, the AERONET AE has two peaks which are not captured well by either of the satellite retrievals. Nevertheless, the ABI Ångström Exponent retrievals meet the F&PS requirement of 0.3 for accuracy, as seen in Table 4-5. Neither of the satellite retrievals of AE meets the requirement for precision (0.15).

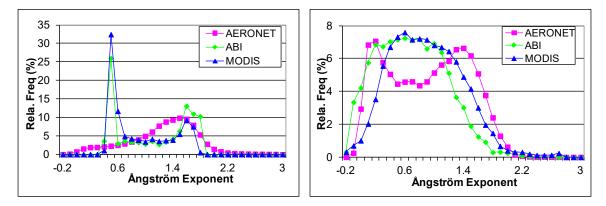


Figure 4-7. Comparison of ABI Ångström Exponent with AERONET over land (left) and over ocean (right) using collocated AERONET-MODIS dataset for years 2000-2012.

Table 4-5. Accuracy and precision of Ångström Exponent retrieval from collocated AERONET-MODIS dataset for years 2000-2012.

	La	nd	Water		
	Accuracy	Accuracy Precision Accuracy I		Precision	
ABI	-0.14	0.57	-0.21	0.40	
MODIS	-0.32	0.53	-0.01	0.36	

### 4.2.1.3 Preliminary evaluation of AOD derived from actual ABI data

AOD was retrieved over selected AERONET sites from reflectance data from ABI onboard GOES 16 using the Version 6.1 algorithm for the period of 04/29/2017-01/15/2018. The resulting ABI-AERONET matchup data then was used to get a preliminary estimate of the algorithm performance. The results are shown for high-quality AOD retrievals within the range [-0.05;+5.00] for land and water in the form of scatter plots in Figure 4-8. The overall bias and standard deviation of the over-land retrieval of ABI AODs relative to the reference AERONET values are 0.04 and 0.12; those for the over-water retrievals are 0.01 and 0.04, both indicating a positive bias. Accuracy and precision broken down into the required AOD ranges are summarized in Table 4-6. As indicated by the values in this table accuracy and precision of ABI AOD estimates meet the requirements except for precision in the high AOD (>0.8) range, where it is almost twice as large as the requirement. The estimate of precision 0.65 is however may not be statistically robust due to the relatively small number of matchups (254).

Land			Water				
AOD range	Accuracy	Precision	# of points	AOD range	Accuracy	Precision	# of points
<0.04	0.02 (0.06)	0.07 (0.13)	4,591	<0.4	0.01 (0.02)	0.04 (0.15)	6,758
0.04 - 0.8	0.04 (0.04)	0.11 (0.25)	38,694				
> 0.8	-0.10 (0.12)	0.65 (0.35)	254	>0.4	-0.003(0.10)	0.11 (0.23)	54

Table 4-6. Accuracy of precision values from evaluations of high-quality 550-nm ABI AOD (range: -0.05 - +5.00) for land and water.

Numbers in parenthesis are the F&PS requirement values.

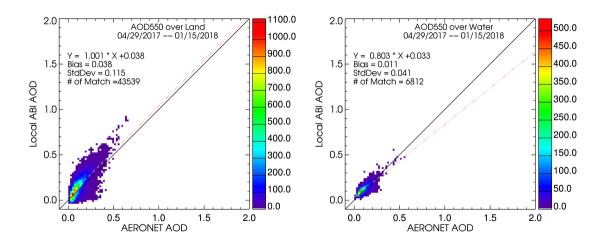


Figure 4-8. Scatter plot of high-quality ABI AOD vs. AERONET AOD for land (left) and water (right) retrieved for the period of 04/29/2017-01/15/2018. The solid black line is the 1-to-1 line; the red dash-dotted line is the linear fit. Slope a and offset b of the linear fit are shown in the fit equation Y=a\*X+b.

#### 4.2.1.4 Framework validation using MODIS radiance

The aerosol algorithm validation discussed in Section 4.2.1.1 and 4.2.1.2 was conducted for the AWG's science code. The science code was integrated into AIT's Framework, and the AIT prepared the algorithm inputs for framework runs on 1-km resolution using MODIS reflectances as proxy data, which included the L1b reflectance, geolocation data, cloud mask, water vapor and ozone from MODIS; and surface pressure, surface height, and surface wind speed/direction from NCEP.

One granule of MODIS data for 03:25 UTC on June 4, 2005 was used to verify the implementation of the algorithm in AIT's framework on a Linux machine within the collaborative environment. The results from the AIT and the AWG runs were compared

and confirmed on a pixel by pixel basis (Figure 4-9). The maximum difference is on the order of 1.0E-6 over land and 1.0E-4 over ocean, and the data with difference larger than 1.0E-6 is about ~ 0.015%. The difference is believed to be the result of the different compilers used; AIT uses the Intel complier, while AWG uses  $g^{++}$ .

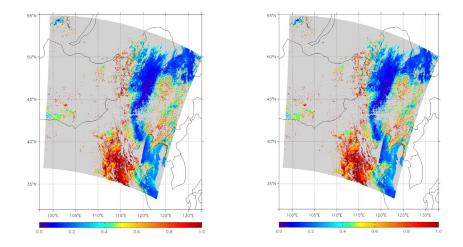


Figure 4-9. Aerosol optical depths at 550 nm, for one MODIS granule at 03:25 UTC on June 4, 2005, generated by the AIT framework run (left) and the AWG research code (right).

At the time the test was conducted data from two days (Aug. 24 and Aug. 25, 2006) were available for analysis. For the analysis of the framework results with AERONET, the AERONET data were averaged within a one-hour window and the collocated ABI estimates were spatially averaged for a 50km  $\times$  50 km region. Following the approach used in the offline validation, the highest 50% and lowest 20% of AODs in the 50  $\times$  50 km boxes were screened out, and the rest were averaged for comparison with AERONET.

Figure 4-10 shows, as a scatter-plot, the comparison between ABI AODs with AERONET measurements at 550 nm over land and water. The overall statistics, including the accuracy, precision and correlation coefficients are presented. The data are also averaged over different AOD ranges to see the dependence of accuracy and precision on AOD as shown in Table 4-7. Note that the match-up points from the two days are quite limited, especially over water, and the statistics cannot be considered representative.

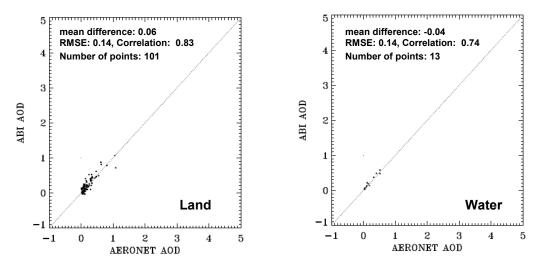


Figure 4-10. Comparison of framework ABI AOD with AERONET AOD at 550 nm over land and over water from 2-day framework run of Aug. 24-25, 2006.

Table 4-7. Accuracy and precision for different AOD ranges from 2-day framework run.

	Land					Water		
Range	AOD	Accuracy	Precision	# of points	AOD	Accuracy	Precision	# of points
Low	< 0.04	0.09	0.01	16		-0.03	0.02	10
Medium	0.04 - 0.8	0.06	0.03	82	<0.4			
High	> 0.8	-0.04	0.01	3	>0.4	-0.05	0.02	3

### 4.2.2 Error Budget

The atmosphere and surface input parameters required for the ABI aerosol retrieval algorithm have associated uncertainties. This section explores the effect of these uncertainties on the retrieved aerosol properties. For this, the input parameters are perturbed (changed) by expected rages of the uncertainties, and the retrieved aerosol properties are compared to the results from retrievals with unperturbed inputs.

TOA reflectances are simulated with the 6S RTM covering a wide range of geometries and aerosol conditions (Table 4-8). Unless otherwise stated, the climatology water vapor (2.0 cm), ozone (380 Dobson units), fixed wind (6 m/s, westerly) are used in the simulation and retrieval processes. The sensitivity experiments for varying parameters are listed in Table 4-9. For each sensitivity test, the values listed in Table 4-9 are used in the forward simulation and a systematic perturbation is applied to the input (for example,  $\pm 8\%$  for the ozone test). The retrieved aerosol products are then compared with those without perturbation in the input (used as reference). Ozone and water vapor are ABI products and

the uncertainty levels used are from their product specifications. Cloud contamination is assumed to increase the TOA reflectance in all ABI channels by 5% or 10%. Surface pressure and ocean surface wind speed/direction are from NCEP data, and the perturbation for surface pressure is assumed as 3% and wind direction as  $10^{\circ}$  for simplicity. The NCEP wind speed is strongly influenced by observed SSM/I (special sensor microwave imager) data; and the algorithm used to derive wind speed has an RMS error of 1.65 m/s compared with buoys for observations peaking in the 4-7 m/s range [Kalnay et al., 1995; Krasnopolsky et al., 1995]. Taking 6 m/s as the mean value, this RMS difference leads to an uncertainty of ~25%.

	Parameters	Dimension	Values
	cosine of solar zenith	10	from 0.4 to 1.0 with a constant
	angle		interval of 1/15
Geometry	cosine of local zenith	10	from 0.4 to 1.0 with a constant
	angle		interval of 1/15
	relative azimuth angle	10	from 0° to 180° with a constant
			interval of 20°
Aerosol op	tical depth at 0.55µm	7	0.1, 0.2, 0.4, 0.6, 0.8, 1.0, 1.5
	Fine mode	4	four fine modes same as those
Aerosol			in the retrieval algorithm
models	coarse mode	5	five coarse modes same as
(ocean			those in the retrieval algorithm
only)	Fine mode weight	6	0, 0.2, 0.4, 0.6, 0.8, 1.0
Aerosol mo	odels (land only)	4	dust, generic, urban, heavy
			smoke same those in the
			retrieval algorithm
Land surface	ce reflectance at 2.25um	10	from 0.02 to 0.2 with a
(land only)			constant interval of 0.02

Table 4-9. Uncertainty levels and values of input atmospheric and surface parameters

Parameters	<b>Uncertainty level</b>	Values
Ozone	+8%	$0.095, 0.19, 0.38, 0.76 (\times 10^3)$
	-8%	Dobson units)
Water vapor	+9%	0.5, 1.0, 2.0, 4.0, 8.0 (cm)
	-9%	
Surface pressure	+3%	standard surface pressure 1013 (hPa)
	-3%	
Cloud contamination	+5%	Modify TOA reflectance at all ABI
	-5%	channel
Surface wind speed	+25%	1.5, 3, 6, 9, 12 (m/s)
(ocean only)	-25%	
	10°	30, 60, 90, 120, 150 (°)

Surface wind	-10°	
direction (ocean		
only)		

The multi-channel aerosol algorithm retrieves aerosol optical depth (AOD), aerosol model and fine-mode weight (FMW) over ocean. A perturbation can change the AOD value, as well as the aerosol model selection and FMW due to the complex multi-channel interdependencies. Figure 4-11 shows the mean value and standard deviation of relative

AOD uncertainty (defined as  $\frac{test - reference}{reference}$  for AOD at 550nm) versus AOD over land

and over water, respectively. The relative AOD uncertainly is larger at low AOD values and smallest for middle AOD values, except for the 'dust in SWIR' case that is discussed later. Among all tests, the aerosol retrieval is the least sensitive to the change in wind direction and therefore not included in Figure 4-11, where the overall relative AOD and FMW uncertainty are within 0.03%, and the model misidentification rate is ~0.8%. In the ocean algorithm, wind direction is fixed as westerly in the LUT, and the test of  $\pm 10^{\circ}$  change only modifies the sunglint directional reflectance.

In Figure 4-11, the uncertainty is generally smaller over ocean than over land mainly because the ocean aerosol retrieval uses more ABI channels, and some channels with less sensitivity to the specified change will weaken the overall effect. The results for the cloud contamination test and wind speed is not displayed in Figure 4-11 due to their relatively large influence as listed in Table 4-10. The aerosol algorithm is less sensitive to uncertainty in ozone and water vapor, suggesting the use of climatology data may be reasonable when the ABI products are missing. However, it is more sensitive to surface pressure, ocean wind speed, and especially cloud contamination, suggesting a need for high quality for those inputs. Over water, the uncertainty due to cloud contamination is expected to be smaller because the specified absolute perturbation is larger for the same percentage level change over land. The percentage of aerosol model misidentification over land is illustrated in Figure 4-12. Based on the results shown in this figure the algorithm can meet specification (11%) for differentiating dust from non-dust aerosols. The FMW uncertainties (defined as *test – control*) over water are generally within 0.05 except for cloud contamination at the 10% level, as shown in Figure 4-13.

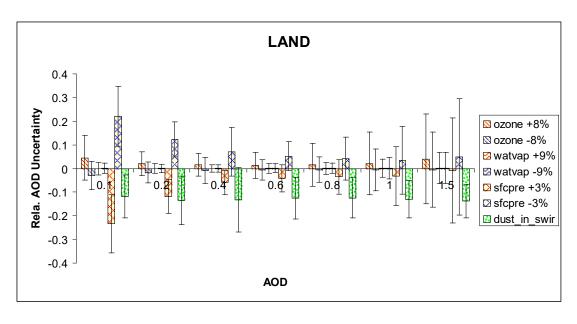
	LAND			WATER			
AOD550	cloud +5%	cloud +10%	cloud +5%	cloud +10%	wspd +25%	wspd -25%	
Bias							
0.1	0.4939	1.0128	0.1168	0.2357	-0.1580	0.0963	
0.2	0.3010	0.5952	0.0643	0.1472	-0.0813	0.0478	

Table 4-10. Mean values and standard deviations of relative AOD errors due to cloud contamination and error in wind speed. (AOD550: aerosol optical depth at 550 nm; wspd: wind speed)

0.4	0.2155	0.4527	0.0531	0.1098	-0.0401	0.0213
0.6	0.1826	0.4097	0.0581	0.1109	-0.0241	0.0124
0.8	0.1743	0.4181	0.0631	0.1207	-0.0163	0.0081
1.0	0.1794	0.4414	0.0649	0.1279	-0.0118	0.0054
1.5	0.1714	0.4217	0.0715	0.1472	-0.0059	0.0025
		Sta	ndard devia	tion		
0.1	0.2372	0.4976	0.1646	0.2401	0.2512	0.1818
0.2	0.2173	0.5043	0.1215	0.1812	0.144	0.0945
0.4	0.2232	0.4463	0.0869	0.1352	0.0816	0.0485
0.6	0.1398	0.3904	0.0777	0.1474	0.0544	0.0324
0.8	0.2050	0.4378	0.0744	0.1468	0.0411	0.0253
1.0	0.2763	0.4700	0.0822	0.1524	0.0323	0.0194
1.5	0.3167	0.3816	0.0859	0.1507	0.0194	0.0111

Underestimating (or neglecting) aerosol scattering in the SWIR channel may introduce large errors for dust particles. To quantify this error, scattering by dust aerosol in all ABI channels (including the SWIR channel) is accounted for in the forward simulation that provides the input TOA reflectances, but not in the retrieval process. The results are then compared with the case of no dust in the forward simulation or in the retrieval process. Underestimating dust in the SWIR channel increases the surface reflectance in this channel and hence those in the red and blue channels, which results in the underestimation of AOD by 10-15% for different AOD values (denoted as 'dust in swir' test in Figure 4-13) and the dust misidentification rate is about 11%.

Doubling/halving of chlorophyll concentration, used in the ocean reflectance model, slightly changes ( $\sim 0.0003$ ) the water-leaving radiance at 0.64µm. However, the effect is so small that it does not change the selection of model combination and FMW from the minimum residual calculation, and hence do not modify the AOD retrieval from the reference channel.



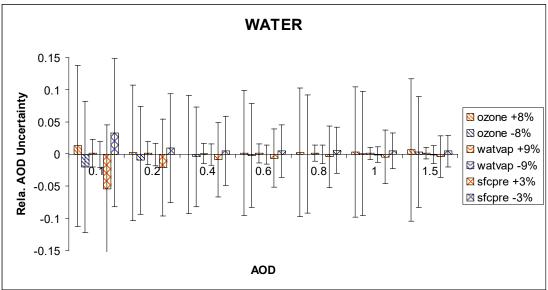


Figure 4-11. Mean values and standard deviations of relative AOD uncertainty for uncertainties in ozone, water vapor (watvap) and surface pressure (sfcpre) over land and water, and dust presence test in SWIR channel (dust in swir) over land.

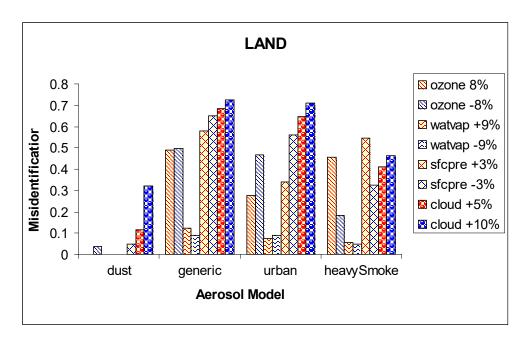


Figure 4-12. Land aerosol model misidentification for ozone, water vapor (watvap), surface pressure (sfcpre) and cloud contamination (cloud) tests.

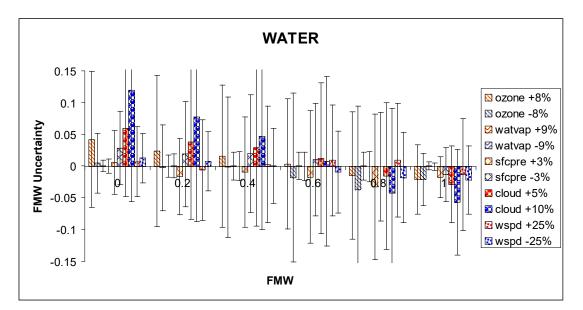


Figure 4-13. Mean values and standard deviations of fine-mode weight (FMW) uncertainty over water for ozone, water vapor (watvap), surface pressure (sfcpre), cloud contamination (cloud), and surface wind speed (wspd) tests.

# **5 PRACTICAL CONSIDERATIONS**

# 5.1 Numerical Computation Considerations

The LUT approach uses pre-calculated values of spectral atmospheric transmittances, reflectances, spherical albedo and surface BRDF as functions of AOD at 550 nm, aerosol models, geometries and ocean surface wind speeds. In the LUT, following the VIIRS approach [Vermote et al., 2006], the TOA is given as a function of scattering angle with an interval of 4 degrees. The range of scattering angles is calculated from the solar and local zenith angles and the relative azimuth angle. This method provides a relatively rapid search of the LUT. Just like in the standard MODIS algorithm [Remer et al., 2005], the interval halving method is used in LUT for searching for the "best" combination of fine and coarse mode of ocean aerosol models; this increases efficiency as well.

# 5.2 **Programming and Procedural Considerations**

The aerosol retrieval is carried out pixel by pixel. It requires calibrated and geo-located ABI reflectances, ABI cloud mask and snow/ice mask as ABI dynamic input. Mapping processes for static ancillary (e.g. surface elevation) can be processed offline. The programming design uses modules, providing the flexibility for ease upgrades.

The data that need to be configurable for possible post-launch adjustment include algorithm coefficients (LUT and land surface reflectance relationship), criterion values (e.g. selecting atmospheric conditions), water vapor and ozone dataset depending on the ABI data availability, and metadata setting.

# 5.3 Quality Assessment and Diagnostics

The following flags will be produced:

- Missing/No data
- Coast, Snow/Ice, Cloud proximity
- Cloud (retrieval from "possibly clear" reflectance category)
- Pixel with large local zenith angle (> 60 degrees)
- Less than maximum number of channels used for retrieval
- Large solar zenith angles
- Negative retrievals
- Retrievals over bright surfaces
- Flags based on spatial variability tests for residual cloud contamination

# 5.4 Exception Handling

The quality control flags for aerosol retrieval will be checked and inherited from the flagged Level 1b sensor input data, including bad sensor input data, missing sensor input data and validity of each aerosol channel; and will be checked and inherited from the ABI cloud mask at each pixel for clear, possibly clear, cloud and possibly cloudy.

The algorithm does checks for conditions not favorable for aerosol retrieval and generates quality control flags for snow/ice pixel, bright surface, nearby cloud and costal pixel, and viewing geometry.

# 5.5 Algorithm Validation

During the pre-launch phase of development, and testing, the primary means of aerosol product validation is the comparison with measurements made from the ground such as AERONET. Because of the limited number of ground locations where high quality ground observations of aerosol properties are made this type of validation is necessarily restricted in space. Evaluation is also done by performing retrievals from model-simulated proxy ABI data, and by comparing the retrieved aerosol product to the known aerosol data used in the simulation. This type of validation is ideal for evaluating algorithm performance not only for the aerosol products but also for all other (input, internal, and ancillary) parameters that influence aerosol retrievals. Because all relevant data are know in the simulations uncovering algorithm (programming) problems is also relatively easy. However, due to the excessive computational burden realization of a wide range of realistic scenarios may not be practical, and thus the validation may be limited in scope. Comparison with (independent) satellite-based aerosol products tests the consistency of ABI retrievals under realistic conditions. To be useful this type of evaluation should be performed for long (preferably continuous) time periods. For this purpose, routine comparisons are carried out by running the ABI retrieval algorithm with near-real time MODIS L1-B radiance data, and then comparing to MODIS products, which are considered to be independent.

Once the actual (final) spectral response functions of the ABI sensors are known or updated the atmosphere and ocean surface LUTs must be re-generated, and the relationship between VIS and SWIR surface reflectances must be re-derived. The validation methodologies listed above will be applied to actual aerosol products.

Validation of the current (Version 6.1) algorithm is presented in Section 4.2. The detailed aerosol products validation is described in the GOES-R aerosol product validation plan documents.

# 6 ASSUMPTIONS AND LIMITATIONS

This section describes the limitations and assumptions in the current version of the aerosol retrieval algorithm, and potential future enhancements to the algorithm.

# 6.1 Performance

The following assumptions have been made in the current algorithm developing:

- Aerosol shape is spherical. Accounting for the non-spherical shape of dust aerosol is studied in a separate and independent research; the results of that research may be included in the retrieval in the future.
- Aerosol is vertically well-mixed, and the impact of aerosol height may not be a priority because the ABI channels for aerosol retrieval are well selected to minimize gas absorption.
- Surface reflectance of ocean can be calculated and that of land can be estimated with sufficient accuracy;
- Land surface is dark and Lambertian. In an AWG sponsored project, an alternative algorithm is currently being developed that may extend the retrievals for bright surfaces. This algorithm does not assume Lambertian surface reflectance. Instead, bidirectional surface reflectance and aerosol optical depth are simultaneously retrieved.
- Calibrated and geo-located radiances in ABI channels 1-6 are available.
- ABI cloud mask is available.
- Ancillary data are available.

The limitations in the current retrieval algorithm are:

- Retrieval limited to dark surface;
- Retrieval limited to clear-sky conditions;
- Retrieval limited to daytime only;
- Retrievals may not be valid at certain viewing geometry.

The 2.25- $\mu$ m channel is critical for the over-land algorithm. Without this channel surface reflectance cannot be estimated and aerosol retrieval is not performed. Loss of either of the 0.47- $\mu$ m or the 0.64- $\mu$ m channel would degrade the performance, since aerosol type cannot be retrieved in this case. Loss of any of the channels used in the over-ocean retrieval would likely lead to decrease of quality. No mitigation against channel loss is implemented in the current (Version 5) algorithm.

## 6.2 Assumed Sensor Performance

The calibrated and geo-located ABI channel radiances are assumed to be available for the current aerosol retrieval algorithm. Over land, loss of 2.25  $\mu$ m channel will disable the algorithm as it is needed to estimate surface reflectance. Similarly, aerosol type cannot be estimated in case the 0.47- or 0.64- $\mu$ m channel is missing. Over ocean, loss of one or two channels of 0.64, 0.86, 1.61 and 2.25  $\mu$ m increases the bias to be about twice of the base case with four channels.

### 6.3 **Pre-Planned Product Improvements**

### 6.3.1 Retrieval over bright land surface

An alternate land algorithm, the Multiangle Implementation of Atmospheric Correction algorithm, MAIAC (Lyapustin et al., 2011a,b, 2012) was initially considered to replace the current over-land algorithm. MAIAC is designed to work over most surface types including bright surfaces (except snow). MAIAC uses the time sequence of images, and thus takes advantage of geostationary geometry of fixed local zenith angle and changing solar zenith angle in a way that allows the simultaneous retrieval of AOD and surface bidirectional reflectance.

Recently, however, a method that extends AOD retrieval from VIIRS to bright, snow-free surfaces was developed (Zhang et al., 2016). The method has been implemented in the NOAA Enterprise Processing System (EPS) aerosol optical depth retrieval algorithm (EPS ATBD, 2016). The EPS AOD algorithm was designed to be capable of making AOD retrievals from either VIIRS or ABI reflectances using a common, consistent algorithm. The bright-surface method in the EPS algorithm works similarly to the dark-surface retrievals except for ABI it uses ratios of 0.47  $\mu$ m to 0.64  $\mu$ m surface reflectances derived for fixed 0.1°x0.1° grids over bright surfaces.

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# APPENDIX

## A. Effect of Instrument noise on AOD Retrieval

The effect of this instrument noise on the retrieved aerosol optical depth is estimated from the Signal-to-Noise Ratio (SNR) following Tanre et al. (1997). In that method a SNR is defined in terms of aerosol optical depth as  $\tau/\Delta\tau$ , where  $\tau$  is the "typical" value of the aerosol optical depth, and the 'Noise Equivalent Differential Optical Depth'  $\Delta\tau$  is estimated using the single-scattering approximation:

$$\Delta \tau = \Delta \rho \frac{4\cos(\theta_v)\cos(\theta_s)}{\omega_0 P(\Theta)},\tag{A-1}$$

where  $\theta_v$  and  $\theta_s$  are solar and local zenith angles,  $\omega_0$  is the aerosol single scattering albedo,  $P(\Theta)$  is the aerosol phase function, and  $\Delta \rho$  is the 'Noise Equivalent Differential Spectral Reflectance' calculated from the SNR for reflectances. Note that different aerosol models have different optical properties ( $\omega_0$ , P) leading to different, aerosol-model dependent sensitivities.

These reflectances are listed in Table A-1 for the required resolution of 2 km for the aerosol retrieval channels. It is noted that the noise for the 0.64- $\mu$ m channel at 500 m resolution is 1/1000, instead of 1/300, because a SNR of 50:1 must be achieved for targets of 5% reflectance, as specified in PORD. (For a detector with SNR=300 for target of 100% reflectance, the noise is 0.33% (in reflectance units). If the noise is also 0.33% for a target of 5% reflectance, the SNR will be 5% / 0.33% = 15. Therefore the noise is assumed to be 0.1%, which means SNR=50 at 5% and SNR=1000 at 100%.)

The largest noise in aerosol optical depth  $\Delta \tau$  is expected for the Sun at zenith ( $\theta_s = 0$ )

and for nadir observation  $\theta_{\nu} = 0$ , and for the lowest value of phase function at a scattering angle of 120° (Tanre et al., 1997; Shettle and Fenn, 1979). The single-scattering albedo and phase function are calculated using nine ocean aerosol models used in the ABI aerosol retrieval (four fine modes and five coarse modes, see Section 3.4.1.2). The resulting  $\Delta \tau$  is listed in Table A-2. Typical values of the spectral aerosol optical thickness  $\tau$  are taken from Hoppel et al., (1990) and also shown in Table A-1. From these values the SNR at 2 km resolution is then calculated. The results for ocean appear in Table A-3.

Channel	0.47 µm	0.64 µm	0.86 µm	1.61 µm	2.25 μm
Noise in Reflectance	1/600	1/4000	1/600	1/600	1/300
at 2km					
Typical τ	0.2	0.1	0.05	0.03	0.01

Table A-1.  $\Delta \rho$  and  $\tau$  for the ABI "aerosol" channels.

Channel	0.47 µm	0.64 µm	0.86 µm	1.61 µm	2.25 μm
F1	0.033	0.003	0.015	0.014	0.033
F2	0.050	0.006	0.031	0.019	0.030
F3	0.064	0.008	0.042	0.023	0.034
F4	0.070	0.009	0.051	0.029	0.041
C1	0.083	0.012	0.082	0.085	0.153
C2	0.096	0.013	0.080	0.085	0.170
C3	0.118	0.014	0.083	0.082	0.170
C4	0.097	0.010	0.055	0.058	0.112
C5	0.118	0.012	0.068	0.063	0.116

Table A-2. Aerosol optical depth sensitivity  $\Delta \tau$  for ABI ocean aerosol models.

Table A-3. Signal-to-noise ratio for optical depth for ocean aerosol models at 2-km resolution.

Channel	0.47 μm	0.64 µm	0.86 µm	1.61 µm	2.25 μm
F1	6.01	32.07	3.32	2.08	0.30
F2	4.02	16.49	1.62	1.56	0.33
F3	3.11	12.23	1.18	1.30	0.30
F4	2.87	10.65	0.98	1.04	0.25
C1	2.40	8.36	0.61	0.35	0.07
C2	2.09	8.00	0.63	0.35	0.06
C3	1.69	7.16	0.60	0.36	0.06
C4	2.05	10.20	0.91	0.52	0.09
C5	1.69	8.40	0.74	0.47	0.09

The optical properties of land aerosol models are assumed to be functions of the optical depth in the ABI aerosol algorithm. However, to simplify estimating the effect of noise in the over-land retrieval the single typical  $\tau$  values in Table A-1 are used again. The signal-to-noise ratios in terms of aerosol optical depth for the land aerosol models are shown in Table A-4.

Table A-4. Signal-to-noise ratio of optical depth for land aerosol models at 2-km resolution.

Channel	0.47 μm	0.64 µm	0.86 µm	1.61 µm	2.25 μm
Smoke	4.23	19.21	1.83	0.65	0.09
Dust	4.84	18.66	1.58	0.86	0.13
Generic	3.59	16.96	1.68	0.63	0.09
Urban	3.21	15.11	1.65	0.66	0.09

The SNRs for optical depth in Table A-3 and Table A-4 indicate that the noise at the 2-km resolution may be too large for accurate aerosol retrieval from ABI channels with

wavelengths of 0.86  $\mu$ m and higher. In terms of this SNR, retrievals might be better performed from the 0.64- $\mu$ m channel where the optical-depth SNRs are 7 or larger. Decreasing the resolution from 2 km to 4 km decreases the noise by a factor of 2, and hence increases the SNR by a factor of 2, and so on. The SNR at different resolutions are shown for the least sensitive (2.25- $\mu$ m) channel for ocean and land aerosol models in Table A-5 and Table A-6, respectively. These results show that the SNR is close to or larger than unity for the 2.25- $\mu$ m channel for all aerosol models when the spatial resolution increases to 32 km. It should be emphasized again that aerosol retrieval in the ABI algorithm is effectively done from the shorter wavelength channels (reference channels of 0.47  $\mu$ m for land, and 0.86  $\mu$ m for ocean) where the SNRs are higher.

Resolution	2 km	4 km	8 km	16 km	32 km
F1	0.30	0.60	1.20	2.39	4.78
F2	0.33	0.66	1.32	2.65	5.30
F3	0.30	0.59	1.19	2.37	4.75
F4	0.25	0.49	0.98	1.97	3.94
C1	0.07	0.13	0.26	0.52	1.05
C2	0.06	0.12	0.24	0.47	0.94
C3	0.06	0.12	0.23	0.47	0.94
C4	0.09	0.18	0.36	0.71	1.43
C5	0.09	0.17	0.35	0.69	1.38

Table A-5. Aerosol optical depth signal-to-noise ratio for ocean aerosol models at  $2.25 \ \mu m$  for different spatial resolutions.

Table A-6. Aerosol optical depth signal-to-noise ratio for land aerosol models at  $2.25 \mu m$  for different spatial resolutions.

Resolution	2 km	4 km	8 km	16 km	32 km
Smoke	0.09	0.17	0.34	0.78	1.38
Dust	0.13	0.26	0.53	1.19	2.12
Generic	0.09	0.17	0.35	0.78	1.38
Urban	0.09	0.19	0.37	0.84	1.49

The above analysis assumes the noise is constant and always present at the same level. A more appropriate interpretation of the SNR values in Table 2-5 is to treat the noise as a random process with a mean of zero and standard deviation of the SNR. In this model the reflectance error is  $\Delta \rho = \mu_o^{-1} N(0, \sigma)$ , where  $\mu_0$  is the cosine of the solar zenith angle, and N is the random noise with standard deviation  $\sigma$  whose values are the SNRs listed in Table 2.5. The effect of the noise on the optical depth retrieval was estimated using this noise

model by performing the ABI aerosol retrieval once from noise free reflectances ( $\sigma = 0$ ) and once with noisy reflectances ( $\sigma = SNR$ ). The reflectances used for this exercise were the MODIS collection 5 10-km aerosol reflectances for 03/2000-12/2007 for Terra and 07/2002 -12/2007 for Aqua. (The MODIS reflectances were assumed to be noise free in this exercise.) Taking the difference of the two retrievals provided a measure of the impact of noise. The retrievals from both reflectances were then compared to collocated AERONET version 2 level 2.0 aerosol data; accuracies and precisions were calculated, which in turn were compared to the requirements. The results indicated only small biases ( $3x10^{-5}-5x10^{-3}$ ) and standard deviations of the biases (0.049) as a result of the assumed noise.

The effect of noise was also evaluated by perturbing the radiance by a constant noise at the level specified in Table A-1. In this exercise the perturbed reflectance  $\rho'_{\lambda}$  is expressed as

$$\mu_0 \rho_{\lambda} = \mu_0 \rho_{\lambda} + Noise \tag{A-2}$$

Here  $\mu_0$  is cosine of solar zenith angle;  $\rho_{\lambda}$  is the un-perturbed TOA reflectance. The TOA ABI reflectances in the aerosol channels were calculated from forward simulation for sample locations selected within the GOES East and West domains with local zenith angles less than 60°. For the east domain 31 locations were specified over ocean and 10 over land. For the west domain 39 locations were used over ocean and 3 over land. The locations are shown in Figure A-1.

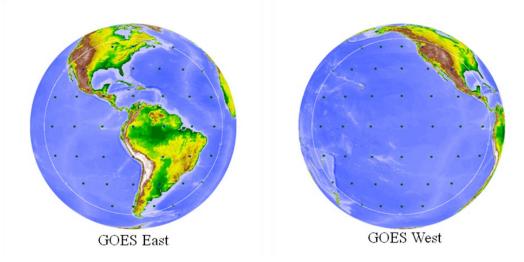


Figure A-1. Locations selected for aerosol retrievals in the GOES east and west domains.

Solar and local zenith and azimuth angles were calculated for every hour of four days (Mar 20, Jun 21, Sep 22, and Dec 21 (solstices and equinoxes)). Solar zenith angles were restricted to be less than 80°. Constant values of total precipitable water (2.0 cm), column ozone amount (0.38 atm-cm), surface elevation (sea level), surface pressure (1013 mb),

wind speed (6 m/s), and wind direction (due east) were assumed. Aerosol models and optical depths and surface albedo over land were as follows:

- Over water
  - 4 fine mode aerosol types
  - 5 coarse mode aerosol types
  - 6 fine mode weight: 0.0, 0.2, 0.4, 0.6, 0.8, 1.0
  - 9 aerosol optical depth at 0.55µm: 0.05, 0.1, 0.2, 0.3, 0.4, 0.6, 0.8, 1.0
- Over land
  - 4 aerosol models: dust, generic, urban, smoke
  - 9 aerosol optical depth at 0.55μm: 0.05, 0.1, 0.2, 0.3, 0.4, 0.6, 0.8, 1.0
  - 10 surface albedo at 2.26  $\mu m$ : 0.02, 0.04, 0.06, 0.08, 0.10, 0.12, 0.14, 0.16, 0.18, 0.20

Retrievals were performed from 1) reflectances without noise; 2) reflectances with positive noise added; and 3) reflectances with negative noise added. The AOD retrieved from the perturbed (nose added) reflectances were then compared to those retrieved from the unperturbed ones, and the aerosol optical depth at  $0.55\mu m$  and Ångström Exponent were analyzed to evaluate the impact of noise. The results are shown in Table A-7, Table A-8, Table A-9, and Table A-10.

Input	Positive Noise Added			Negative Noise Added			
AOD	Bias	Std. dev	Number	Bias	Std. dev	Number	
0.05	0.007	0.016	276120	0.010	0.025	51878	
0.1	-0.002	0.024	276120	0.013	0.031	132643	
0.15	-0.009	0.030	276120	0.017	0.036	180733	
0.2	-0.015	0.037	276120	0.020	0.041	206434	
0.3	-0.025	0.052	276120	0.026	0.054	228493	
0.4	-0.031	0.067	276120	0.027	0.080	241682	
0.6	-0.039	0.103	276120	0.027	0.123	259060	
0.8	-0.037	0.155	276120	0.033	0.171	264795	
1.0	-0.031	0.211	276120	0.042	0.220	267165	

Table A-7. Bias and standard deviation (Std.dev) of AOD retrieved over water from noisy reflectances relative to that from noise-free reflectance.

The results in Table A-7 show that adding positive/negative specified noise leads to, on average, negative/positive biases in the retrieved AOD. These are somewhat unexpected since one would think that an increased TOA reflectance would lead to an increase in the retrieved AOD. The counter-intuitive results can be attributed to the dynamic selection of aerosol model (fine/coarse aerosol types and fine mode weight). As shown in , perturbing the TOA reflectance by adding noise changes the spectral shape of reflectances. As a result, larger/smaller aerosol model is selected when the positive/negative noise is added. Due to

different aerosol models being selected, increasing/decreasing TOA reflectance can lead to smaller/larger AOD being retrieved, and the impact increases as the input AOD increases.

		Ångströ	m Exponent	(0.47-0.86	μm)	
Input	Posit	ive Noise A	Added	Ne	gative Noise A	Added
AOD	Bias	Std. dev	Number	Bias	Std. dev	Number
0.05	-0.611	0.543	276120	0.700	0.552	51878
0.1	-0.308	0.396	276120	0.424	0.371	132643
0.15	-0.166	0.328	276120	0.334	0.334	180733
0.2	-0.091	0.281	276120	0.274	0.300	206434
0.3	-0.025	0.249	276120	0.200	0.237	228493
0.4	-0.012	0.231	276120	0.160	0.207	241682
0.6	-0.008	0.214	276120	0.122	0.179	259060
0.8	-0.008	0.186	276120	0.097	0.157	264795
1.0	-0.008	0.167	276120	0.081	0.143	267165
		Ångströ	m Exponent	(0.86-2.13	μm)	
Input	Posit	ive Noise A	dded	Ne	gative Noise A	Added
AOD	Bias	Std. dev	Number	Bias	Std. dev	Number
0.05	-0.810	0.853	276120	0.791	0.643	51878
0.1	-0.685	0.778	276120	0.613	0.530	132643
0.15	-0.602	0.724	276120	0.537	0.518	180733
0.2	-0.543	0.685	276120	0.462	0.487	206434
0.3	-0.465	0.638	276120	0.348	0.429	228493
0.4	-0.405	0.602	276120	0.259	0.368	241682
0.6	-0.322	0.523	276120	0.152	0.336	259060
0.8	-0.258	0.436	276120	0.113	0.294	264795
1.0	-0.224	0.384	276120	0.102	0.230	267165

Table A-8. Bias and standard deviation (Std.dev) of the Ångström Exponent retrieved over water from noisy reflectance relative to that from noise-free reflectance.

Table A-9. Bias and standard deviation (Std.dev) of AOD retrieved over land from noisy reflectances relative to that from noise-free reflectance.

Input	Positive Noise Added			Negative Noise Added		
AOD	Bias	Std. dev	Number	Bias	Std. dev	Number
0.05	0.017	0.010	21880	-0.016	0.009	21816
0.1	0.016	0.013	21880	-0.012	0.016	21816

0.15	0.015	0.018	21880	-0.009	0.020	21816
0.2	0.016	0.022	21880	-0.012	0.021	21816
0.3	0.025	0.111	21880	-0.016	0.028	21816
0.4	0.035	0.176	21880	-0.016	0.049	21816
0.6	0.038	0.149	21880	-0.017	0.060	21816
0.8	0.041	0.202	21880	-0.017	0.106	21816
1.0	0.054	0.359	21880	-0.006	0.263	21816

Table A-10. Bias and standard deviation (Std.dev) of the Ångström Exponent retrieved over land from noisy reflectance relative to that from noise-free reflectance.

		Ångströ	m Exponent	(0.47-0.86	μm)		
Input	Posi	tive Noise A	dded	Negative Noise Added			
AOD	Bias	Std. dev	Number	Bias	Std. dev	Number	
0.05	0.296	0.402	21880	-0.597	0.420	21816	
0.1	0.285	0.436	21880	-0.664	0.537	21816	
0.15	0.263	0.434	21880	-0.443	0.567	21816	
0.2	0.215	0.404	21880	-0.223	0.461	21816	
0.3	0.121	0.300	21880	-0.058	0.259	21816	
0.4	0.067	0.211	21880	-0.032	0.210	21816	
0.6	0.038	0.191	21880	-0.019	0.188	21816	
0.8	0.010	0.180	21880	-0.015	0.193	21816	
1.0	-0.018	0.159	21880	-0.011	0.206	21816	
		Ångströ	m Exponent	(0.86-2.13	μm)		
Input	Posi	tive Noise A	dded	Ne	gative Noise A	Added	
AOD	Ring	Std dov	Number	Ring	Std dov	Number	

Input	Positive Noise Added			Negative Noise Added		
AOD	Bias	Std. dev	Number	Bias	Std. dev	Number
0.05	0.253	0.323	21880	-0.488	0.338	21816
0.1	0.253	0.361	21880	-0.545	0.441	21816
0.15	0.244	0.377	21880	-0.368	0.487	21816
0.2	0.210	0.372	21880	-0.180	0.432	21816
0.3	0.130	0.308	21880	-0.021	0.288	21816
0.4	0.074	0.251	21880	0.010	0.262	21816
0.6	0.029	0.259	21880	0.023	0.243	21816
0.8	-0.008	0.267	21880	0.019	0.236	21816
1.0	-0.224	0.384	276120	0.102	0.230	267165

The results presented in the tables above indicate that effects of perturbing TOA reflectance with noise on the aerosol retrieval are three-fold:

- Increasing/decreasing TOA reflectance in the reference channel (0.86 μm for water and 0.47 μm for land) directly leads to higher/lower AOD being retrieved (if same aerosol model is used).
- 2. The change of spectral shape of TOA reflectance leads to different aerosol models being selected.
- 3. Over land, change of TOA reflectance at SWIR channel affects the estimated surface reflectance.

As a result, the impact on the retrieved AOD is not straightforward. As shown in the tests over water, an increase of TOA reflectance leads to decreased AOD on average.

Defining the Signal-to-Noise Ratio in terms of AOD (SNR-AOD) as the ratio of input AOD over the standard deviation of retrieval error, it is seen that for a typical AOD value of 0.15 over water, the SNR-AOD is  $\sim$  5. Over land, for a typical value of 0.2, the SNR-AOD is  $\sim$ 10. These SNR-AOD values suggest that the noise for the 2-km "pixel" is small enough to retrieve an AOD.

### **B.** Sunglint directional reflectance

In calculating the reflectance of water Cox and Munk (1954) considered the system of coordinates (P,X,Y,Z) where P is the observed point, Z the altitude, PY is pointed to the sun direction and PX to the direction perpendicular to the sun plane. Using spherical trigonometry, the components of surface slope  $Z_x$  and  $Z_y$  which is so inclined to reflect an incoming ray from the sun toward the satellite can be related to the sun-satellite geometry through:

$$Z_{X} = \frac{-\sin(\theta_{v})\sin(\phi_{s} - \phi_{v})}{\cos(\theta_{s}) + \cos(\theta_{v})};$$

$$(B-1)$$

$$\sin(\theta_{v}) + \sin(\theta_{v})\cos(\phi_{v} - \phi_{v})$$

$$Z_{Y} = \frac{\sin(\sigma_{s}) + \sin(\sigma_{v})\cos(\varphi_{s} - \varphi_{v})}{\cos(\theta_{s}) + \cos(\theta_{v})}$$
(B-2)

To simplify the calculation, the (P,X,Y) coordinate system is rotated to a new set of principal axes (P, X', Y') with PY' parallel to the wind direction. The slope components are now expressed as:

$$Z'_{\chi} = \cos(\chi) Z_{\chi} + \sin(\chi) Z_{\gamma}; \qquad (B-3)$$

$$Z'_{Y} = -\sin(\chi)Z_{X} + \cos(\chi)Z_{Y}, \qquad (B-4)$$

where  $\chi$  is the relative azimuth angle between sun and wind direction. The possibility for the occurrence of such slope is calculated as:

$$p(Z'_{X}, Z'_{Y}) = (2\pi\sigma'_{X}\sigma'_{Y})^{-1} \exp\left(-\frac{\xi^{2} + \eta^{2}}{2}\right)$$

$$\times \begin{cases} 1 - \frac{1}{2}C_{21}(\xi^{2} - 1)\eta - \frac{1}{6}C_{03}(\eta^{3} - 3\eta) + \frac{1}{24}C_{40}(\xi^{4} - 6\xi^{2} + 3) + \\ \frac{1}{4}C_{22}(\xi^{2} - 1)(\eta^{2} - 1) + \frac{1}{24}C_{04}(\eta^{4} - 6\eta^{2} + 3) \end{cases}$$
(B-5)

where  $\xi = \frac{Z'_X}{\sigma_X}$  and  $\eta = \frac{Z'_Y}{\sigma_Y}$ .  $\sigma'_X$  and  $\sigma'_Y$  are the root mean square values of  $Z'_X$ and Z' the elements of finitum C and C and the nonlocal square values of  $Z'_X$ 

and  $Z'_{y}$ , the skewness coefficients  $C_{21}$  and  $C_{03}$ , and the peakedness coefficients  $C_{40}$ ,  $C_{22}$ and  $C_{04}$  have been defined by Cox and Munk for a clean surface as follows:

$$\sigma_X^{\prime 2} = 0.003 + 0.00192 ws; \quad \sigma_Y^{\prime 2} = 0.00316 ws$$

$$C_{21} = 0.01 - 0.0086 ws; \quad C_{03} = 0.04 - 0.033 ws$$

$$C_{40} = 0.40, \quad C_{22} = 0.12; \quad C_{04} = 0.23,$$

where WS is the wind speed with a lower limit set as 0.1 m/s to ensure numerical stability.

The directional reflectance is written as:

$$\rho_{sgt}(\theta_s, \theta_v, \phi_s, \phi_v) = \frac{\pi \cdot p(Z_X, Z_Y) \cdot R(n_r, n_i, \theta_s, \theta_v, \phi_s, \phi_v)}{4 \cdot \cos \theta_s \cdot \cos \theta_v \cdot \cos^4 \beta}, \quad (B-6)$$
  
where  $\beta$  is the tilt  $(\tan \beta = \sqrt{Z_X^2 + Z_Y^2}).$ 

Fresnel's reflection Coefficient  $R(nr, ni, \theta_s, \theta_v, \phi_x, \phi_v)$  is computed as:  $R(nr, ni, \theta_s, \theta_v, \phi_s, \phi_v) = \frac{1}{2} \left\{ \frac{\left[ (n_r^2 - n_i^2) \cos \theta_i - u \right]^2 + \left[ 2n_r n_i \cos \theta_i + v \right]^2}{\left[ (n_r^2 - n_i^2) \cos \theta_i + u \right]^2 + \left[ 2n_r n_i \cos \theta_i - v \right]^2} + \frac{(\cos \theta_i - u)^2 + v^2}{(\cos \theta_i + u)^2 + v^2} \right\}$ (B-7) where,

$$u^{2} = \frac{1}{2} \left\{ \left| n_{r}^{2} - n_{i}^{2} - \sin^{2} \theta_{i} \right| + \sqrt{\left( n_{r}^{2} - n_{i}^{2} - \sin^{2} \theta_{i} \right)^{2} + 4n_{r}^{2} n_{i}^{2}} \right\}$$

$$v^{2} = \frac{1}{2} \left\{ -\left| n_{r}^{2} - n_{i}^{2} - \sin^{2} \theta_{i} \right| + \sqrt{\left( n_{r}^{2} - n_{i}^{2} - \sin^{2} \theta_{i} \right)^{2} + 4n_{r}^{2} n_{i}^{2}} \right\}$$

$$\cos \theta_{i} = \sqrt{\frac{1}{2} \left[ 1 + \cos \theta_{s} \cos \theta_{v} + \sin \theta_{s} \sin \theta_{v} \cos(\phi_{s} - \phi_{v}) \right]}$$

$$\sin \theta_{i} = \sqrt{\frac{1}{2} \left[ 1 - \cos \theta_{s} \cos \theta_{v} - \sin \theta_{s} \sin \theta_{v} \cos(\phi_{s} - \phi_{v}) \right]}$$

Normalized integral of downward diffuse radiation by sunglint directional reflectance  $\overline{\rho_{sgt}}$  is pre-calculated using the 6S RTM and stored in LUT for varying geometry (solar zenith angle, local zenith angle, and relative azimuth (sun – satellite)), aerosol model and optical

depth, and surface wind speed (see section 3.4.4).  $\overline{\rho'_{sgt}}$  is the normalized integral of upward diffuse radiation by sunglint directional reflectance and can be obtained from the same LUT as  $\overline{\rho_{sgt}}$  by swapping solar zenith and local zenith angles. Linear interpolation is used for intermediate values of arguments from LUT. Noted that wind direction is fixed when calculating  $\overline{\rho_{sgt}}$  and  $\overline{\rho'_{sgt}}$  in the glint LUT, but not for explicit calculation of specular reflection (calculated with analytical Fresnel Equation).

The sunglint spherical albedo  $\overline{\rho_{sgt}}$  is also calculated following 6S RTM. In each ABI channel, the sunglint spherical albedo decreases with wind speed from 2 to 14 m/s by about 5%, therefore it is parameterized as a function of surface wind speed.

# C. Versions of GOES-R AOD algorithm

In this section, versions of operational GOES-R AOD algorithm updates are listed in Table C-1.

Version of algorithm	Date of	Updates
	implementation	
Version 6.1	07/24/2018	Provisional maturity update including GOES-16 land surface relationship update, 2 km resolution of input ABI channel reflectances, etc.
Version 6.2	09/04/2020	Aerosol Particle Size Parameter over water added to the product file
Version 6.3	10/23/2020	Updates on land surface relationships for GOES-16 and GOES-17, as well as GOES-17 look-up-tables
Version 6.4	Unknown	GOES-18 look-up-tables delivered to PRO team on 04/22/2022

Table C-2: Versions of operational GOES-R AOD algorithm update

# **Appendix D: Common Ancillary Data Sets**

### 1. LAND\_MASK\_NASA\_1KM

#### a. Data description

Description: Global 1km land/water used for MODIS collection 5

Filename: lw\_geo\_2001001\_v03m.nc Origin: Created by SSEC/CIMSS based on NASA MODIS collection 5 Size: 890 MB. Static/Dynamic: Static

#### b. Interpolation description

The closest point is used for each satellite pixel:

- 1) Given ancillary grid of large size than satellite grid
- 2) In Latitude / Longitude space, use the ancillary data closest to the satellite pixel.

### 2. MDS\_L2\_CLD\_MASK\_FILE

#### a. Data description

Description: MODIS L2 cloud mask 1km Filename: MOD35\_L2.AYYYYDDD.HHMM.005.yyyydddhhmmss.nc / MYD35\_L2.AYYYYDDD.HHMM.005.yyyydddhhmmss.nc. Where, MOD35\_L2/MYD35\_L2 - Level 2 Cloud Mask from TERRA (MOD) /

AQUA (MYD)

A – Nothing to do here YYYYDDD – 4 digit year plus 3 digit of Julian day HHMM – 2 digit of hour and 2 digit of minutes in GMT 005 – Processing system version yyyydddhhmmss – processing date/time Origin: NASA DAAC Size: 45 MB Static/Dynamic: Dynamic

#### b. Interpolation description

The closest point is used for each satellite pixel:

In Latitude / Longitude space, use the ancillary data closest to the satellite pixel.

### 3. MDS\_L2\_OZON\_5KM\_FILE

#### a. Data description

Description: MODIS L2 ozone 5km Filename: MOD07\_L2.AYYYYDDD.HHMM.005.yyyydddhhmmss.nc / MYD07\_L2.AYYYYDDD.HHMM.005.yyyydddhhmmss.nc. Where, MOD07\_L2/MYD07\_L2 – Level 2 Product Name from TERRA (MOD) / AQUA (MYD)

A – Nothing to do here YYYYDDD – 4 digit year plus 3 digit of Julian day HHMM – 2 digit of hour and 2 digit of minutes in GMT 005 – Processing system version yyyydddhhmmss – processing date/time Origin: NASA DAAC Size: 31 MB Static/Dynamic: Dynamic

#### b. Interpolation description

The closest point is used for each satellite pixel:

In Latitude / Longitude space, use the ancillary data closest to the satellite pixel.

### 4. MDS\_L2\_TPW\_5KM\_FILE

#### a. Data description

Description: MODIS L2 TPW 5km Filename: MOD07\_L2.AYYYYDDD.HHMM.005.yyyydddhhmmss.nc / MYD07\_L2.AYYYYDDD.HHMM.005.yyyydddhhmmss.nc. Where, MOD07\_L2/MYD07\_L2 – Level 2 Product Name from TERRA (MOD) / AQUA (MYD) A – Nothing to do here

A – Nothing to do here
YYYYDDD – 4 digit year plus 3 digit of Julian day
HHMM – 2 digit of hour and 2 digit of minutes in GMT
005 – Processing system version
yyyydddhhmmss – processing date/time

Origin: NASA DAAC Size: 31 MB Static/Dynamic: Dynamic

### b. Interpolation description

The closest point is used for each satellite pixel:

In Latitude / Longitude space, use the ancillary data closest to the satellite pixel.

#### 5. NWP\_GFS

#### a. Data description

Description: NCEP GFS model data in grib format – 1 x 1 degree (360x181), 26 levels Filename: gfs.tHHz.pgrbfhh Where, HH – Forecast time in hour: 00, 06, 12, 18 hh – Previous hours used to make forecast: 00, 03, 06, 09 Origin: NCEP Size: 26MB Static/Dynamic: Dynamic

#### b. Interpolation description

There are three interpolations are installed:

NWP forecast interpolation from different forecast time:

Load two NWP grib files which are for two different forecast time and interpolate to the satellite time using linear interpolation with time difference.

Suppose:

T1, T2 are NWP forecast time, T is satellite observation time, and T1 < T < T2. Y is any NWP field. Then field Y at satellite observation time T is:

Y(T) = Y(T1) \* W(T1) + Y(T2) \* W(T2)

Where W is weight and

W(T1) = 1 - (T-T1) / (T2-T1)W(T2) = (T-T1) / (T2-T1)

NWP forecast spatial interpolation from NWP forecast grid points. This interpolation generates the NWP forecast for the satellite pixel from the NWP forecast grid dataset.

The closest point is used for each satellite pixel:

- 1) Given NWP forecast grid of large size than satellite grid
- 2) In Latitude / Longitude space, use the ancillary data closest to the satellite pixel.

#### NWP forecast profile vertical interpolation

Interpolate NWP GFS profile from 26 pressure levels to 101 pressure levels

For vertical profile interpolation, linear interpolation with Log pressure is used:

Suppose:

y is temperature or water vapor at 26 levels, and y101 is temperature or water vapor at 101 levels. p is any pressure level between p(i) and p(i-1), with p(i-1) . <math>y(i) and y(i-1) are y at pressure level p(i)and p(i-1). Then y101 at pressure p level is:

 $y_{101}(p) = y(i-1) + \log(p[i] / p[i-1]) * (y[i] - y[i-1]) / \log(p[i] / p[i-1]))$ 

### 6. SFC\_ELEV\_GLOBE\_1KM

#### a. Data description

**Description:** Digital surface elevation at 1km resolution. **Filename:** GLOBE\_1km\_digelev.nc **Origin:** NGDC Size: 1843.2 MB Static/Dynamic: Static

### b. Interpolation description

The closest point is used for each satellite pixel:

- 1) Given ancillary grid of large size than satellite grid
- 2) In Latitude / Longitude space, use the ancillary data closest to the satellite pixel.

# 7. SNOW\_MASK\_IMS\_SSMI

### a. Data description

Description: Snow/Ice mask, IMS – Northern Hemisphere, SSM/I – Southern Hemisphere 4km resolution – the 25 km SSM/I has been oversampled to 4km Filename: snow\_map\_4km\_YYMMDD.nc Origin: CIMSS/SSEC Size: 39 MB. Static/Dynamic: Dynamic

### b. Interpolation description

The closest point is used for each satellite pixel:

- 1) Given ancillary grid of large size than satellite grid
- 2) In Latitude / Longitude space, use the ancillary data closest to the satellite pixel.