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2	Refining aerosol optical depth retrievals over land by constructing
3	the relationship of spectral surface reflectances through deep
4	learning: application to Himawari-8
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6	Tianning Su ¹ , Istvan Laszlo ^{2,1} , Zhanqing Li ¹ , Jing Wei ¹ , Satya Kalluri ²
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8	¹ Department of Atmospheric and Oceanic Science and ESSIC, University of Marylan
9	d, College Park, Maryland 20740, USA
10	² Center for Satellite Applications and Research, NOAA/NESDIS,
11	College Park, Maryland 20740, USA

Abstract

For the past two decades, quantitative retrievals of aerosol optical depth (AOD) have 13 14 been made from both geostationary and polar-orbiting satellites, and the results have been widely used in numerous studies. Despite the progress made in improving the 15 16 accuracy of AOD retrievals, there are still major challenges, especially over land. A notable one for the so-called Dark-Target (DT) algorithms is building the surface 17 reflectance (SR) relationships (SRR) to derive SR in the visible channels from SR in 18 the short-wave infrared (SWIR) channel, mainly because these relationships are 19 20 strongly subjected to entangled factors (e.g., viewing geometry, surface type, and vegetation state). In this study, we examine the benefits of a new method for deriving 21 the SRR using deep learning techniques. The SRR constructed by the deep neural 22 23 network (DNN) considers multiple related inputs, such as the SWIR normalized difference vegetation index (NDVI_{SWIR}), viewing geometry, and seasonality, among 24 others. We then incorporate the DNN-constrained SRR into a DT algorithm developed 25 at NOAA/STAR to retrieve AOD from the Advanced Himawari Instrument (AHI) 26 onboard the new generation of geostationary satellites, Himawari-8. The revised DT 27 algorithm with the deep learning technique (DTDL) demonstrates improved 28 performance over the study region (95–125°E, 18–30°N, a portion of the AHI full disk), 29 as attested by significantly reduced random noise, especially for low NDVI_{SWIR} and 30 high surface albedo cases. Robust independent tests indicate that this algorithm can be 31 applied to untrained regions, not only to those used in training. The method directly 32 benefits the algorithm development for Himawari-8 and can also be adopted for other 33

- 34 geostationary or polar-orbiting satellites. Our study illustrates how artificial intelligence
- 35 could significantly improve AOD retrievals from multi-spectral satellite observations
- 36 following this new approach.

37 **1. Introduction**

Aerosols critically impact Earth's climate through modulating the energy budget 38 39 and cloud properties and serve as the primary source of uncertainties to quantifications and interpretations of the changing radiation budget of Earth (Ackerman et al., 2004; 40 Boucher et al., 2013; Chung et al., 2012; Guo et al., 2017, 2019; Li et al., 2011, 2017; 41 42 Ramanathan et al., 2001). To qualitatively and quantitatively understand aerosols' impact on the climate system, measuring aerosol optical properties using advanced 43 remote sensing techniques is increasingly needed (Kahn et al., 2017; King et al., 2003; 44 45 Pavlov et al., 2018; Su et al., 2020a; Wei et al., 2018). Among these properties, aerosol 46 optical depth (AOD) is the critical and most widely used product to tackle both scientific questions and air quality monitoring (Chu et al., 2002; Guo et al., 2020; Li et 47 al., 2015; Lin et al., 2015; Su et al., 2017, 2020b; van Donkelaar et al., 2006; Wei et al., 48 2019a, b). This task is especially important and challenging over land due to the 49 complexity of underlying land properties and aerosol types (Gupta et al., 2016; Levy et 50 51 al., 2005; Li et al., 2009).

During the last 20 years, substantial progress has been made in aerosol remote sensing techniques for satellites, which is considered the best way to obtain long-term, large-scale AOD products (Colarco et al., 2010; King et al., 1999; Li et al., 2009). Launched onboard Terra (1999) and onboard Aqua (2002), the Moderate Resolution Imaging Spectroradiometer (MODIS) has offered benchmark global AOD retrievals over a long period, which have been extensively used in numerous studies (Gupta et al., 2016, 2018, 2019; Han et al., 2020; 2018; Kaufman et al., 2005; Levy et al., 2007a; Li et al., 2013; Lin et al., 2016; Remer et al., 2008; Su et al., 2018; Wei et al., 2019c, 2020;
Yu et al., 2006). Following the success of MODIS, measurements from multiple
geostationary and polar-orbiting satellites have been used to retrieve AOD at regional
and global scales (Kahn et al., 2009; Laszlo, 2018; Laszlo et al., 2008, 2020; Yoshida
et al., 2018).

Several algorithms have been developed to retrieve AOD using data from these 64 sensors, with different merits and weaknesses. A widely used algorithm, the Dark 65 Target (DT) algorithm, has been employed in multiple sensors (Jackson et al., 2013; 66 67 Kaufman et al., 1997a; Levy et al., 2007b), which has good performance over low 68 albedo regions (e.g., dark ocean and dark vegetated surfaces) (Levy et al., 2013). Another popular algorithm, the Deep Blue (DB) or ultraviolet method, can provide 69 70 retrievals over bright surfaces with useful accuracy (Hsu et al., 2006, 2013). As a relatively new method, the Multi-Angle Implementation of Atmospheric Correction 71 (MAIAC) has been used to retrieve AOD at the native 1-km resolution with high 72 accuracy (Lyapustin et al., 2011, 2018). Since the DT algorithm was mainly developed 73 74 for relatively dark regions, the DB and MAIAC algorithms offer higher retrieval rates 75 and more accurate retrievals over bright surfaces due to their different strategies (Hsu et al., 2013; Lyapustin et al., 2018). Among these methods for MODIS, the MAIAC-76 derived AOD has the best performance (Liu et al., 2019; Mhawish et al., 2019). 77

The abovementioned algorithms work reasonably well for polar-orbiting satellites,
providing long-term AOD products with extensive coverage. However, the temporal
resolution for polar-orbiting satellites is limited, while geostationary satellites have

great potential to fill this gap (Kim et al., 2008, 2019). An advanced geostationary 81 satellite named Himawari-8 was successfully launched on 7 October 2014 by the Japan 82 83 Meteorological Agency. As a vital sensor onboard Himawari-8, the Advanced Himawari Imager (AHI) provides spectral reflectance measurements every 10 minutes 84 85 with variable spatial resolutions of 0.5–2 km at different channels covering Southeast Asia, East Asia, part of South Asia, and Oceania. With high spatial and temporal 86 resolutions, the AHI offers a great opportunity to continuously monitor aerosols over 87 Asia in detail (Gupta et al., 2019). Nevertheless, recent studies have revealed that 88 89 Himawari-8 AOD products from the Japan Meteorological Agency still suffer from large uncertainties, especially for low Normalized Difference Vegetation Index (NDVI) 90 cases (Wei et al., 2019d; Zhang et al., 2019). 91

92 In this study, we focus on improving the DT algorithm, as implemented with Himawari-8/AHI observations at the Center for Satellite Applications and Research 93 (STAR), National Oceanic and Atmospheric Administration (NOAA) (Laszlo et al., 94 2008, 2018a, 2018b). A core part of the DT algorithms is the estimation of spectral 95 surface reflectances (SR) in the visible channels (0.47/0.64 µm) from SR in the short-96 97 wave infrared (SWIR) channel (2.25 µm). The usual way to accomplish this is to use 98 empirical functions to describe the SR relationships (SRR) between the visible and SWIR channels with consideration of the scattering angle and the NDVI at SWIR 99 (NDVI_{SWIR}) (e.g., Jackson et al., 2013; Kaufman et al., 1997b; Levy et al., 2007b). Due 100 to the complexity of the SR relationships, such empirical regressions usually lead to 101 102 relationships fraught with large biases, a major source of uncertainties in AOD

103 retrievals.

Since it appears difficult to establish mathematical functions in closed form that 104 105 accurately characterize the SRR, deep learning techniques may offer a better way to deal with the task. The multi-layer artificial neural network, a primitive deep learning 106 technique, has been widely employed (Cireşan et al., 2012; Liu et al., 2017; Seide et al., 107 2011) for a variety of environmental and geographical studies (e.g., Deng and Yu, 2014; 108 Ma et al., 2020; Tong et al., 2019). Hence, we use the multi-layer neural network (i.e., 109 the deep neural network, or DNN) to construct the SRR that accounts for the influences 110 of multiple variables (*NDVI_{SWIR}*, viewing geometry, time, etc.). The DNN-constrained 111 112 SRR is then incorporated into the NOAA/STAR DT algorithm. The revised DT algorithm with deep learning techniques (DTDL) provides an example of how deep 113 learning could improve retrievals of AOD from multi-spectral satellite observations. 114 The paper is structured as follows: General information about multi-source data 115 used and preprocessing are presented in Section 2. Section 3 describes the SRR 116 117 constructed by traditional fitting and by the DNN. Section 4 presents the methodology of the revised algorithm DTDL. The objective of this paper is to test the application of 118

a deep learning technique for deriving SRR and to demonstrate the improvement in

AOD retrievals. Therefore, we only present the most relevant features of the algorithm
in Section 4. An evaluation of the new algorithm is demonstrated in Section 5. Section
6 presents a summary and concluding remarks.

124 **2. Data and Instruments**

125 2.1. Himawari-8/AHI sensor

126 The new generation of geostationary satellite Himawari-8 carrying AHI was launched on 7 October 2014 and became operational on 7 July 2015. AHI is able to 127 image East Asia every 30 seconds while offering full-disk coverage of the Pacific region 128 (longitude: 80°E - 160°W, latitude: 60°S - 60°N) every 10 minutes from a 129 geostationary orbit ~140°E 130 over the equator at (https://www.data.jma.go.jp/mscweb/en/product/library_data). Table S1 summarizes 131 132 the characteristics of the spectral channels of AHI. The NOAA/STAR over-land AOD algorithm uses five shortwave channels (1, 3, 4, 5, and 6) with central wavelengths of 133 0.47, 0.64, 0.86, 1.61, and 2.25 µm. The nominal spatial resolutions of observations in 134 135 these channels are, in order, 1, 0.5, 1, 2, and 2 km. To provide consistent inputs, observations from the higher-resolution channels are averaged to the lowest spatial 136 resolution of 2 km, with a temporal resolution of 30 min. Due to the focus of our current 137 project, we obtained AHI data over a specific region (95–125°E, 18–30°N) in 2017 (see 138 Fig. 1). We analyze data from 00:00 to 09:00 UTC, which corresponds to the daytime 139 over the region studied. 140

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142 2.2. Ground AOD measurements

In this study, we utilize ground-based AOD datasets obtained from two observation
networks: the Aerosol Robotic Network (AERONET) and the Chinese Sun–Sky
Radiometer Observation Network (SONET). The ground-based observation network of

sun and sky scanning radiometer, AERONET, provides aerosol retrievals under clear-146 sky conditions every 15 min. It is widely utilized to evaluate aerosol retrievals derived 147 148 from satellites (Giles et al., 2019; Holben et al., 1998; Li et al., 2014). With reported uncertainties of 0.01-0.02, AOD retrievals derived from AERONET are much more 149 accurate than any satellite retrieval (Eck et al., 1999) and have thus been regarded as 150 "ground-truth". Version 3 Level 1.5 AOD products derived from AERONET are used 151 in our study (https://aeronet.gsfc.nasa.gov/). The ground-based CIMEL radiometer 152 network in China, SONET (http://www.sonet.ac.cn/), uses the same instruments and 153 154 algorithms as used in AERONET, with a similar uncertainty of 0.01-0.02 (Li et al., 2018). 155

Here, we used data from 16 AERONET sites and 2 SONET sites for cloud-free 156 157 scenes over the study region (Fig. 1). The AERONET and SONET AOD retrievals are typically available at multiple wavelengths (i.e., 440, 500, 675, 870, and 1020 nm). 158 Following Eck et al. (1999), a quadratic fit is used to characterize the relationship 159 between the logarithm of AOD and the logarithm of wavelength. The AOD at 550 nm 160 is then interpolated, based on the relationship between AOD and wavelength. The 161 ground-based AODs at 550 nm are used in two ways. They provide the AOD input 162 needed to estimate the SR from which the SRR is built (see Section 3.1). They are also 163 the source of "ground-truth" in the evaluation of AHI-retrieved AOD (see Section 5). 164

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166 2.3. Auxiliary data

167 An external cloud mask serves as input for identifying clear-sky pixels for both

establishing the SRR and aerosol retrievals. The external cloud mask (Heidinger et al., 168 2016) is produced upstream to the AOD retrieval, and as such, it is not part of the AOD 169 170 algorithm. The cloud mask is processed at the same temporal and spatial resolutions as the AHI measurements. Note that the presence of cirrus clouds in a scene is usually 171 172 detected by the 1.38-µm channel in other satellites (Gao et al., 1995, 2002). Due to the lack of a 1.38-µm channel on AHI, cirrus is primarily identified by the 11- and 12-µm 173 split-window test. We note that other methods also exist for detecting cirrus in an AHI 174 pixel. For example, Imai and Yoshida (2016) developed a CO₂ slicing technique. We 175 176 also use the land/ocean mask to choose the appropriate algorithm (land or ocean) for retrieving AOD. 177

Total amounts of water vapor and ozone, surface wind field, pressure, and surface 178 altitude are obtained at a horizontal resolution of $0.5^{\circ} \times 0.5^{\circ}$ from the National Centers 179 for Environmental Prediction Global Forecast System (GFS) model data at a 3-hr 180 (https://www.nco.ncep.noaa.gov/pmb/products/gfs/). interval These 181 data are interpolated to match the uniform spatial resolution of 2 km and the temporal resolution 182 of 30 min of the AHI reflectance data. In particular, model data are linearly interpolated 183 to match the times of satellite observations. For a given satellite pixel, we use the model 184 data closest to the pixel. The temporal and spatial resolutions of GFS data are coarser 185 than those of the satellite data. Thus, interpolation inevitably leads to some uncertainties. 186 Note that the model itself also suffers from considerable uncertainties. However, since 187 observations are not available everywhere, the only feasible option is using model or 188 reanalysis data. 189

191 **3.** Spectral surface reflectance relationships

SR estimated by SRR is one of the most important factors affecting the accuracy of 192 AOD retrievals over land (Kaufman et al., 1997b; Levy et al., 2007b). Similar to the 193 DT algorithm for MODIS (Remer et al., 2005), the National Environmental Satellite, 194 Data, and Information Service/STAR DT algorithm (Laszlo et al., 2018a) retrieves SR 195 (simultaneously with AOD) using empirical relationships between the SRs in the blue 196 (0.47 µm), red (0.64 µm), and SWIR (2.25 µm) bands of dark, dense vegetation. 197 198 Kaufman et al. (1997b) explained that the existence of such relationships is the result of the correlation between chlorophyll (which absorbs radiation in the red/blue band) 199 and liquid water (which absorbs radiation in the SWIR band). 200

The estimation of spectral SR needed to build the relationships is described next. This is followed by showing "traditional" regression-based relationships and an improved relationship derived by applying a deep neural network.

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205 *3.1. Estimation of SR*

SRs at 0.47, 0.64, and 2.25 μ m needed to determine the relationships between them are estimated from the AHI reflectances by accounting for atmospheric effects. Following Vermote et al. (1997a), we use the NOAA/STAR DT AOD algorithm that calculates the surface and atmospheric contributions to the top-of-the-atmosphere (TOA) reflectance. Assuming a Lambertian surface, contributions of the surface (ρ_{surf}) and atmosphere (ρ_{atm}) to the TOA reflectance (ρ_{toa}) are calculated as (Vermote et al., 212 1997a, 1997b):

213
$$\rho_{surf} = T^{O_3} T^{Og} T^{H_2 O} \left[T_{R+A} T_{R+A} \frac{\rho_{lam}}{1 - S_{R+A} \rho_{lam}} \right]$$
(1)

214
$$\rho_{atm} = T^{O_3} T^{og} \left[\left(\rho_{R+A} - \rho_R(P_0) \right) T^{\frac{1}{2}H_2O} + \rho_R(P) \right]$$
(2)

215
$$\rho_{toa} = \rho_{atm} + \rho_{surf} \tag{3}$$

where T^{og} indicates the transmittance from absorption contributed by gases other than 216 $T^{O_{3}}$ represents the transmittance from ozone water vapor and ozone; 217 absorption; T^{H_2O} and $T^{\frac{1}{2}H_2O}$ are the transmittances from total and half column water 218 vapor absorption, respectively; T_{R+A}/T_{R+A} indicate the total (i.e., direct plus diffuse) 219 downward/upward atmospheric transmissions; S_{R+A} represents the atmospheric 220 spherical albedo; $\rho_R(P)$ represents the Rayleigh reflectance contributed by molecular 221 scattering at the real surface pressure (P); ρ_{R+A} represents the path reflectance by 222 molecules and aerosols at the standard surface pressure (P_0); and ρ_{lam} is the 223 Lambertian land surface reflectance. When everything needed to calculate ρ_{atm} is 224 known, ρ_{surf} is determined from Eq. 3. Equation 2 is then solved for the surface 225 reflectance ρ_{lam} . We apply this process at the AERONET/SONET sites where AOD is 226 known from ground-based measurements. 227

Radiative properties of aerosols (normalized extinction coefficient, phase function, and single-scattering albedo) required to calculate reflectances and transmittances are currently prescribed by one of four candidate aerosol models (generic, urban, smoke, and dust) identified by the NOAA/STAR DT algorithm as part of the AOD retrieval. We recognize that this aerosol model may not be optimal for two reasons. First, the candidate models only represent broad categories of aerosol properties. For a particular

retrieval, the actual property of aerosols likely differs from the property prescribed by 234 any of the candidate models. Second, since the model selection is influenced by the 235 236 SRR used in the DT algorithm, uncertainties in SRR contribute to the uncertainty in the model selection, especially when the 550-nm AOD is larger than about 0.5, i.e., when 237 238 the radiative properties of candidate aerosol models differ the most from each other. For the dataset used in this study, this applies to only about 30% of the samples. The 239 approximate threshold of 0.5 applies only for the generic and urban models and for the 240 normalized extinction of the smoke model. Radiative properties of dust and the single-241 242 scattering albedo and phase function of smoke are different from those of the generic and urban models, even at optical depths smaller than 0.5. The impact of erroneous 243 model selection is expected to be somewhat mitigated by screening out low-quality 244 245 retrievals, which, among other factors, are associated with poor agreement between the observed and calculated TOA spectral reflectances, which can happen when the aerosol 246 model picked by the retrieval is likely in error. Even though the calculated SR suffers 247 from multiple sources of uncertainties (e.g., the Lambertian assumption, aerosol optical 248 properties, and aerosol vertical distribution), it is still considered suitable for retrieving 249 AOD because the same assumptions are made in the AOD retrieval. Thus the SRs 250 calculated from Eqs. 1-3 are considered as "ground truth". 251

Calculations of $T^{H_2 0}$ and T^{0_3} require the column amounts of water vapor and ozone, respectively. These parameters, along with other meteorological parameters needed in Eq. 1, are obtained from the GFS. Laszlo et al. (2018a) provide details of calculations of all gaseous transmittances, including T^{og} and Rayleigh reflectance. In

- constructing the database used for establishing SRR, all available 2-km SR retrievalsare averaged within 10 km around the ground sites.
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259 3.2 SRR from regression

The absorption of liquid water and chlorophyll at visible (e.g., blue or red bands) and SWIR wavelengths are related to the state of the vegetation. The relationships of spectral SR are also affected by the vegetation state, as well as seasonality (Kaufman and Remer, 1994; Kobayashi et al., 2007; Remer et al., 2001). The state of vegetation is usually characterized by the top-of-canopy NDVI. However, because this NDVI requires knowledge of AOD, $NDVI_{SWIR}$ is used as an aerosol-independent measure of the vegetation state, in practice. It is defined as (Levy et al., 2007b):

267
$$NDVI_{SWIR} = (\rho_{1.61}^m - \rho_{2.25}^m)/(\rho_{1.61}^m + \rho_{2.25}^m)$$
 (4)

where $\rho_{1.61}^{m}$ and $\rho_{2.25}^{m}$ are the AHI-measured reflectances at 1.61 µm (channel 5) and 2.25 µm (channel 6), respectively.

Figure 2 presents the scatterplots of $SR_{0.47}$ (Fig. 2a-b) and $SR_{0.64}$ (Fig. 2c-d) as 270 271 a function of $SR_{2.25}$, with colors representing values of $NDVI_{SWIR}$ (left panels) and 272 scattering angle (right panels). Hereafter, SR_{λ} represents the SR at wavelength λ (i.e., 0.47, 0.64, and 2.25 µm). Despite the scatter, higher SR is generally associated with 273 274 lower NDVI_{SWIR} and higher scattering angles. The simplest linear regressions in the form of Y = m + n X, where m and n are constants, are also shown. These simple linear 275 regressions cannot fully characterize the SRR between visible and SWIR channels, so 276 it is necessary to add NDVI_{SWIR} and scattering angle into the empirical relationship 277

between SR in multiple channels (Laszlo et al., 2018a; Remer et al., 2013). Table 1
presents the SRR obtained this way and used in this study as one of the possible
empirical functions to represent the SRR. The regression coefficients are derived from
the least-squares method for multiple parameters (Bühlmann and Van De Geer, 2011).

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283 *3.3. SRR from DNN*

We adopted the DNN to derive SR at the visible channel (0.64 μ m) from SR at the SWIR channel (2.25 μ m). The DNN is designed based on the structure and functions of the nervous system and the brain, which can contain a large number of interconnected individual elements (i.e., artificial neurons) working in parallel (Cireşan et al., 2012; Sarle, 1994; Seide et al., 2011). Using a sufficient dataset to train the model, a DNN model can provide a predicted output for new input data due to its learning ability (Schmidhuber, 2015).

Instead of specific functions, we use the DNN to train the relationship between 291 $SR_{2,25}$ based on measurements within 10 km around 292 $SR_{0.64}$ and the AERONET/SONET sites. Based on the previous descriptions and Eqs. 1-3, we add 293 additional inputs, including NDVI_{SWIR}, scattering angle, TOA reflectances at 294 0.47/0.64/2.25 µm, seasonality, column amount of ozone, column amount of water 295 vapor, and the pressure at the surface level. Meteorological parameters are obtained 296 from the NCEP GFS. The seasonality is classified as winter (December-January-297 February), spring (March-April-May), summer (June-July-August), and autumn 298 (September-October-November). The four seasons are denoted as 1, 2, 3, and 4, 299

respectively. The seasonality is then used in the DNN training and prediction. Due to 300 the nonlinearity in the relationships among various parameters, the DNN model is based 301 302 on the Bayesian regularization approach for tracking various nonlinear functions (Burden and Winkler, 2008). The maximum number of epochs is set as 10,000 to allow 303 sufficient training. As shown in Fig. 3, the corresponding input data are extracted from 304 a geographical grid. The input data are then interconnected with multiple neurons 305 within the hidden layers. Figure 3 also shows the architecture of neurons in the hidden 306 layers. The total number of hidden layers is n+3, where n can be adjusted as needed. 307 308 The first and second hidden layers have 8 and 4 neurons, respectively, and the last hidden layer has one neuron. Other hidden layers have two neurons. The neuron is a 309 processing element that sums the inputs and weights. The strengths and importance of 310 311 the connections are represented by neuron biases and weights, which are automatically adjusted in the training process. The predicted $SR_{0.64}$ would then be generated for a 312 given grid based on the training model. 313

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315 *3.4. The performance of SRR derived from regression and DNN*

The performance of the empirical function in the traditional approach is shown in Fig. 4a that plots the 0.64- μ m SR estimated from the empirical function as a function of the "true" 0.64- μ m SR obtained from the AHI TOA reflectance and the groundobserved AOD using Eqs. 1–3. The plot shows a fair amount of scatter for individual retrievals that could lead to considerable errors in AOD. The empirical function is also likely to underestimate at the high end and overestimate at the low end of the "true" SR 322 values.

For evaluating the performance of the DNN model, we use the sample-based cross-323 324 validation (CV) technique (Rodriguez et al., 2010). For the CV process, we randomly choose 70% of the total samples for training, then utilize the remaining 30% of the 325 dataset for validation. Such a procedure is repeated ten times to avoid biases in the 326 selection. Basically, the data sample size for validation is expanded ten times, while the 327 samples do not overlap with the training data. Figures 4b-e present the scatterplots of 328 the 10-CV results of $SR_{0.64}$ for different numbers of hidden layers with the 329 330 architecture shown in Fig. 3. Samples of 10-CV are three times the original dataset. The number of neurons is a critical parameter in the DNN but does not significantly affect 331 the DNN performance in this study. Despite a slightly larger bias when the number of 332 333 hidden layers is three, DNN-derived $SR_{0.64}$ shows consistent performance for different numbers of neurons. With the smallest root-mean-square error (RMSE), we 334 set the total number of the hidden layers to 7 and the total number of neurons to 27. In 335 the architecture constructed in our study, the DNN predicts SR_{0.64} with RMSEs and 336 mean absolute errors (MAEs) that are about a third of those predicted by the empirical 337 function, as shown in Fig. 4. 338

Following previous studies (e.g., Gupta et al., 2016), we still use an empirical linear relationship to calculate $SR_{0.47}$ from $SR_{0.64}$ (Fig. S1). The linear regression predicting $SR_{0.47}$ from $SR_{0.64}$ captures the overall, dominant characteristics of the true $SR_{0.47}$ and results in a relatively good correlation coefficient (0.9). But the residual error of the linear fit is still considerable because of the large scatter in the data.

In the current stage, we do not use the DNN to train the relationship between $SR_{0.47}$ 344 from $SR_{0.64}$ because we found that the DNN may predict unphysical values of $SR_{0.47}$ 345 346 based on preliminary analyses (e.g., smaller than 0 or larger than 0.3, the maximum value expected for the vegetated surface at this wavelengths). However, we do not rule 347 out the possibility that the DNN may improve the performance of retrieved $SR_{0.47}$ 348 with appropriate inputs and architecture. Based on the linear fitting of SR, we use a 349 simple regression ($SR_{0.47} = 0.86 \times SR_{0.64} - 0.02$) to derive $SR_{0.47}$ from the DNN-350 derived $SR_{0.64}$. To avoid negative values, $SR_{0.47}$ is set to 0.01 when $SR_{0.64}$ is less 351 352 than 0.025.

353

4. Dark-target – Deep-learning (DTDL) algorithm

4.1. The algorithm combining the DNN and the DT method

We implemented the DNN scheme for the SRR into the NOAA/STAR DT 356 algorithm for Himawari-8/AHI. This DT algorithm follows the approach applied to the 357 358 GOES-R Advanced Baseline Imager and described in more detail by Laszlo et al. (2018a). For this DT algorithm, the land aerosol models are adopted from previous 359 studies for MODIS (Levy et al., 2007a; Remer et al., 2006). Detailed information about 360 these aerosol models can be found in Table S2. There are notable uncertainties in the 361 AOD retrievals associated with assumed aerosol models, which may lead to 362 uncertainties of more than 10% in the retrievals (Jeong et al., 2005; Mielonen et al., 363 2011; Tirelli et al., 2015; Wang et al., 2017; Wu et al., 2016). This is very difficult to 364 solve since we cannot actually obtain or retrieve the real aerosol model from 365

monodirectional, multispectral intensity measurements alone. Moreover, different types
of aerosols are mixed in the real atmosphere and show large vertical variations. Such
complex information may not be conveyed by some common aerosol models (Li et al.,
2020). Unlike oceans, the surface properties of land demonstrate large variability and
great complexity, making modeling the spectral SR difficult. The bias in SR further
serves as a major source of uncertainties in the aerosol retrieval over land. The SRR
trained by the DNN is expected to mitigate the problem.

The retrieval algorithm can be described as searching for the pair of AOD and SR 373 374 that leads to calculated TOA reflectances which best fit the observed TOA reflectances at 0.47, 0.64, and 2.25 µm. Instead of directly using a radiative transfer model (i.e., 6SV 375 v1.1), a look-up table (LUT) of necessary terms for several candidate aerosol models, 376 377 AOD values, and geometries was generated, based on the 6S vector radiative transfer model (Vermote et al., 1997a) for efficient calculations. Figure 5 outlines the procedure 378 of simultaneous AOD retrievals and SR. For each aerosol model, an iterative procedure 379 380 is presented by looping over the AOD values in the LUT in ascending order. For a specific step *i* in the loop, a value of $SR_{2,25}$ is calculated from the AOD and the TOA 381 reflectance in the SWIR channel. $SR_{0.64}$ is then directly estimated through the DNN-382 trained SRR described in Section 3.1.1. $SR_{0.47}$ is calculated from the DNN-derived 383 $SR_{0.64}$, based on linear regression. The TOA reflectance at 0.47-µm ($\rho_{0.47,i}$) is derived 384 from $\tau_{550,i}$ and $SR_{0.47}$. The loop over the AOD values is terminated when $\rho_{0.47,i}$ 385 converges to the observation ($\rho_{0.47}^{obs}$). For the current aerosol model, the AOD retrieval 386 is further estimated based on linear interpolation. Furthermore, the corresponding TOA 387

reflectance at 0.64 μ m is calculated from the current AOD retrieval and $SR_{0.64}$. The associated residual is calculated as the squared difference between the observed TOA reflectance and the calculated TOA reflectance at 0.64 μ m. By looping the aerosol model, the AOD retrieval is selected as the solution with the smallest residual.

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393 *4.2. Quality control*

In the NOAA/STAR DT algorithm, several external masks and internal tests are 394 applied to screen out unsuitable pixels and control the quality of AOD retrievals. Details 395 396 of the procedures are provided by Laszlo et al. (2018a), but here, we summarize the major ones for completeness. First, pixels with $\rho_{0.47}^{obs} > 0.4$ are deemed as cloudy or 397 too bright for the aerosol retrieval and are excluded. An internal snow test and 398 399 ephemeral water test are then applied, following previous studies (Jackson et al., 2013; Walton et al., 1998). An internal inhomogeneity test is also performed to further screen 400 pixels. Detailed information on these tests is provided in the publicly available 401 algorithm theoretical basis documents referenced by Laszlo et al. (2018a). Based on the 402 retrieval residual, external masks, and internal tests, the AOD retrievals are classified 403 into four quality levels (i.e., no retrieval, low quality, medium quality, and high quality). 404 Following Laszlo et al. (2018a), Table S3 summarizes the criteria for determining the 405 quality level of AOD retrievals. Cases with no retrieval and low quality are excluded in 406 our analyses, including those presented in Section 3. 407

408

409 **5. Evaluation of AOD retrievals**

410 5.1. An Overview of AOD retrievals from the DTDL algorithm

411 After implementing the DTDL algorithm, AOD retrievals at 550 nm were made from Himawari-8/AHI over the study region during the period 1 January 2017 to 31 412 December 2017 at a 2-km spatial resolution. To isolate the changes in the retrievals 413 caused by the SRR, retrievals from the DTDL algorithm used the same inputs as the DT 414 algorithm. Figure 6a shows the medium- and high-quality AODs that are used in the 415 evaluation. Several polluted regions associated with high population densities are 416 417 identified with relatively high AOD values, including the Red River Delta, the Sichuan Basin, western Taiwan, and the Pearl River Delta. The available retrieval rate is 418 calculated as the number of available AOD retrievals divided by the total number of 419 420 samples (~3600), which is around 20% for plains with dense vegetation. It is much lower for arid regions due to the relatively brighter surface (Fig. 6b). The spatial 421 distributions of averaged AOD and retrieval rates during daytime for high-quality 422 AODs are presented in Fig. S2. The AOD pattern is similar for high-quality cases in 423 terms of spatial distribution, but the retrieval rates are generally less than one-third of 424 the total sampling. The DTDL algorithm uses the same framework as the DT algorithm. 425 The retrieval rates of the DTDL and the DT algorithms are thus the same when AOD is 426 not filtered for quality. By contrast, algorithms, like the MAIAC algorithm, that provide 427 retrievals over a wide range of surfaces (Mhawish et al., 2019) are expected to have 428 higher retrieval rates than those of the DTDL algorithm. 429

430

We also compare the diurnal variation in AODs retrieved from Himawari-8/AHI

measurements and those derived from ground measurements (Fig. 7). These diurnal 431 variations are averaged from data for the year 2017. AHI retrievals matched with ground 432 433 measurements from 18 sites are used to avoid biases due to sampling differences caused by quality control. The ensemble of all matched data is then used in the analyses of the 434 AOD diurnal variations. In general, aerosol loading based on ground data slightly 435 increases between 00:00-02:00 UTC, reaching a maximum value around 02:00 UTC, 436 and gradually decreasing thereafter. The AHI AOD retrievals derived from the original 437 DT method have a very different diurnal pattern. DT-derived AODs generally decrease 438 439 until about 02:00 UTC, reaching a maximum around 06:00 UTC. As a result, the largest bias exists around 02:00 UTC when the ground AOD reaches its maximum, and the DT-440 derived AOD is much lower. However, the mean bias of DT is not always larger than 441 442 the DTDL bias. For example, it is slightly smaller than that of the DTDL at 05:00 UTC. The diurnal biases for the original DT and the DTDL algorithms during different 443 seasons are presented in Fig. S3. The considerable mean bias of the DT retrievals 444 around 02:00 UTC is likely caused by the large bias during spring (Fig. S3). After 445 implementing the DTDL method, the systematic biases during spring diminish 446 considerably. The AHI AOD retrievals from the DTDL algorithm show higher 447 consistency with the ground AOD measurements in all seasons. Some features in AOD 448 biases are shared by the original DT and DTDL algorithms, such as the overestimation 449 in AOD retrievals at 00:00 UTC. Such systematic biases need to be considered when 450 451 using AHI AOD retrievals in this region.

Figure 8a-b show comparisons between ground-measured AOD and AOD derived 454 455 from the original DT algorithm for medium-quality and high-quality data. Figure 8c-d show comparisons between ground-measured AOD and AOD derived from the DTDL 456 algorithm. Note that 70% of ground AOD measurements used in model training are 457 excluded from the analysis. The AODs retrieved from the DTDL algorithm are 458 generally improved for both medium-quality and high-quality categories. With the new 459 DTDL algorithm, DNN-based SRR, the uncertainties (represented by the MAE) of the 460 AHI retrievals are reduced by about 30%. Such a significant reduction in noise 461 462 considerably improves the quality of the AOD product.

The DTDL method is able to produce better AOD retrievals over a region even 463 464 though the training takes place in another region. Additional independent tests were performed to demonstrate this. The study region was divided into four regions: R1 and 465 R2, defined by latitude, and L1 and L2, defined by longitude (Table 2). We use the 466 467 dataset from R1 to train the model and validate the results over R2. Such a test is repeated for each region. Figure 9a-d shows comparisons between ground-measured 468 AOD and DT-derived AOD for the four regions. Figure 9e-h shows comparisons 469 470 between ground-measured AOD and DTDL-derived AOD for R1, R2, L1, and L2, while the training datasets are obtained over regions R2, R1, L2, and L1, respectively. 471 This process ensures the independence of training and validation datasets. Medium-472 quality and high-quality retrievals are jointly used here. For all four regions, the DTDL-473 derived AOD shows notable improvement in all three metrics used to measure quality 474

(i.e., correlation coefficient, RMSE, and MAE). The uncertainties of AOD retrievals by
DTDL are reduced by 15–25%. The same procedure is performed for high-quality cases,
producing similar results (Fig. S4). Thus, the DTDL algorithm not only performs better
in regions with training data but also consistently performs better than the traditional
DT algorithm over untrained regions.

Regarding the original DT method, the empirical relationship leads to a large bias 480 in estimated SR and can further contribute to the notable uncertainties in AOD retrievals. 481 By implementing a DNN model, multiple contributing factors for the SRR, such as 482 483 meteorological data and seasonality, can be taken into consideration. The DNN model appears to be a good way to characterize the complex and nonlinear SRR between 484 visible and SWIR channels. The accuracy of AOD retrievals considerably benefits from 485 486 the improved SRR derived from the DNN. Many factors contribute towards the biases in AOD retrievals, such as surface reflectance, cloud contamination, aerosol model, and 487 aerosol vertical distribution, among others. In this study, we have focused on refining 488 489 the surface reflectance assumption, but we also bear in mind that other factors can contribute to the error in AOD retrievals. 490

491

492 5.3. Uncertainty related to various factors

Since the quality of satellite AOD retrievals depends on the underlying surface and viewing geometry, we calculate the mean absolute differences between the AOD retrievals from ground measurements and AHI under various conditions. Figure 10 shows the average absolute bias of AOD for different values of $SR_{0.47}$, $SR_{0.64}$,

NDVI_{SWIR}, and scattering angle for medium-quality and high-quality retrievals. The 497 mean absolute biases for the original DT and DTDL algorithms are 0.15 and 0.1, 498 499 respectively. However, the absolute biases in DT-derived AOD can be very large for scenes with a high albedo and low NDVI. This is because the biophysical relationship 500 is valid for dark and dense vegetation but less valid for arid and bright surfaces 501 characterized by low NDVI and a high albedo. Note that the frequency of occurrence 502 of high albedo in the region studied is low. Thus, even relatively few outliers can 503 considerably affect the average calculated from AOD over regions with a high surface 504 505 albedo.

506 Compared with the original DT algorithm, the absolute bias of the DTDL algorithm is systematically reduced under various conditions. In Fig. 10, the shaded parts 507 represent standard deviations that are generally larger for the original DT algorithm 508 than for the DTDL algorithm. The traditional DT method cannot deal well with 509 relatively bright surfaces or less vegetated surfaces. Although the DTDL algorithm is 510 also significantly affected by these factors, the revised method can considerably 511 mitigate this issue. The absolute biases of high-quality retrievals as functions of SR, 512 NDVI_{SWIR}, and scattering angle are presented in Fig. S5. The pattern of change in biases 513 514 with these variables is similar to that shown in Fig. 10 for the combined medium- and high-quality retrievals, but the magnitude of the biases is smaller. The DTDL algorithm 515 also produces smaller absolute biases in AOD retrievals at all 18 sites (Fig. S6). 516

The biases in AOD retrievals are considerably reduced after implementing the DNN-derived SRR in the DTDL algorithm. However, since the visualization of a deep

learning model is generally insufficient, interpretability and casualty have been widely
recognized as major weaknesses of the DNN (Runge et al., 2015; Zhang et al., 2018),
which may be addressed in the future Montavon et al., 2017; Reichstein et al., 2019).
Currently, we only compare the original DT and DTDL algorithms in this study since
there is no public Himawari-8 AOD product from the other two major methods (DB
and MAIAC).

525

526 6. Summary

527 In this paper, we developed a new method (DTDL) that combines the traditional DT approach, as applied in the NOAA/STAR AOD algorithm for AHI, with a deep 528 529 learning technique (i.e., DNN) to improve estimates of spectral SR needed for AOD 530 retrievals. The core part of the algorithm for retrieving AOD is a radiative transfer model represented by a LUT. The DTDL algorithm still keeps this part (i.e., the LUT) 531 but changes how the surface reflectance is estimated. Due to the complexity of land 532 surface properties, the difficulty in modeling spectral SR constitutes a major source of 533 uncertainties in AOD retrievals in the DT algorithm. The DTDL algorithm applies the 534 DNN to infer the surface albedo at the visible channel and to tackle the nonlinear 535 relationship between multiple, mutually dependent parameters. The improvement in 536 characterizing SRR leads to better AOD retrievals. 537

538 One year of the Himawari-8/AHI dataset is employed for the evaluation of the 539 proposed method. The DTDL algorithm demonstrates better performance over the 540 study region, with a ~30% reduction in random noise. AOD retrievals are significantly

affected by the albedo and vegetation state of the underlying surface. Low NDVI and 541 high albedo are associated with each other and are two major factors contributing to 542 543 large biases in AOD retrievals by the DT algorithm. After applying the DNN-derived SRR in the DTDL algorithm, this problem is lessened considerably. Four independent 544 545 tests are carried out to train and test in different regions to ensure the applicability of the DTDL algorithm. The DTDL algorithm consistently produces better retrievals than 546 the traditional DT algorithm over untrained regions, with a ~20% reduction in 547 uncertainties. 548

549 Due to its stability and accuracy, the DTDL algorithm has a large potential for improving aerosol retrievals over land. The comprehensive evaluation provides firm 550 support for our method in the study region. Although this area spans thousands of 551 552 kilometers, it is still limited to a portion of the AHI full disk. The surface measurements of AOD at the 18 sites under study do not cover all underlying surface conditions. 553 Therefore, the application of the DTDL algorithm to a larger area is warranted to gain 554 555 a full understanding of the representation and adaptability of this method. The deep learning technique and strategy may also be revised and improved in the future. 556

As pointed out by Reichstein et al. (2019), a physical scheme and deep learning can be complementary, and their fusion offers great potential for geoscientific analysis. Our study successfully implements this strategy and shows the potential application of such a hybrid method combining the physical approach and deep learning. Our study demonstrates how artificial intelligence could significantly improve AOD retrievals from multi-spectral satellite observations.

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- 924

- 925 List of Tables
- **Table 1.** Empirical functions relating surface reflectances (*SR*) at 0.47, 0.64, and 2.25
- μ m. Θ indicates the scattering angle. *NDVI_{SWIR}* is the shortwave infrared normalized
- 928 difference vegetation index.

NDVI _{SWIR} range	m S	$SR_{0.64} = m$ $n = a + b imes \Theta$ $R_{0.47} = 0.86$	$+ n \times SR$ $n = c - \frac{1}{2}$ $\times SR_{0.64} + \frac{1}{2}$	2.25 + <i>d</i> × Θ − 0.02
	а	b	С	d
NDVI _{SWIR} <0.2	-0.0416	0.00058	0.68	-0.00095
$0.2 \le NDVI_{SWIR} \le 0.3$	-0.038	0.00060	0.9	-0.0036
$0.3 \le NDVI_{SWIR} \le 0.4$	-0.026	0.00026	1.21	I
$0.4 \leq NDVI_{SWIR} < 0.5$	-0.0147	0.000067	1.32	I
$0.5 \le NDVI_{SWIR}$	0.0077	-0.00011	0.91	I

		938
Region code	Classification	Number of sites
R1	Latitude > 23°N	9
R2	Latitude < 23°N	9
L1	Longitude > 110°E	12
L2	Longitude < 110°E	6

Table 2. Classification of different regions for independent tests.



Fig. 1. Spatial distribution of terrain height (unit: m) of the study region. Red dots
indicate the 16 AERONET sites, and pink dots indicate the 2 SONET sites used in our
study.



Fig. 2. (a, b) The linear regression between $SR_{0.47}$ (surface reflectance at 0.47 µm) 963 and $SR_{2.25}$ (surface reflectance at 2.25 µm). (c, d) The linear regression between 964 (surface reflectance at 0.64 μ m) and SR_{2.25}. In (a, c), the color-shaded dots 965 $SR_{0.64}$ indicate the corresponding NDVI_{SWIR}. In (b, d), the color-shaded dots indicate the 966 corresponding scattering angle. The black solid lines and error bars represent the 967 average values and standard deviations for each bin, which divides the x-axis into ten 968 equal parts. The regression equations and correlation coefficients (R) are given at the 969 top of each panel. The SR data are derived from matched ground AOD and AHI data. 970



Fig. 3. Diagram describing the deep neural network (DNN) used to derive $SR_{0.64}$.

 $SR_{0.47}$ is calculated from $SR_{0.64}$, based on a simple linear function (Table 1).



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Fig. 4. (a) Density scatterplots of the comparison between surface reflectance (SR) at 975 $0.64 \,\mu m \,(SR_{0.64})$ predicted by the empirical function and $SR_{0.64}$ calculated from Eqs. 1– 976 3, the "true" surface reflectance. (b-e) Density scatterplots of 10-cross-validation results 977 for $SR_{0.64}$ derived from DNN, considering different numbers of hidden layers in the 978 DNN model. The correlation coefficients (R), root-mean-square errors (RMSE), and 979 mean absolute errors (MAE) are given in each panel. The solid black lines represent the 980 best-fit lines from linear regression. The dashed grey lines are plotted as Y=0.8X and 981 Y=1.2X (positions of 20% error). 982



Fig. 5. Flowchart of the DTDL algorithm for retrieving AOD for clear pixels over land.

- 985 The modules enclosed by the red, dashed lines represent updates the DTDL algorithm
- 986 introduced into the NOAA/STAR DT algorithm.



Fig. 6. Spatial distributions of (a) mean aerosol optical depth (AOD) and (b) available

retrieval rate derived from the DTDL algorithm for the year 2017.



Fig. 7. Diurnal variation in Himawari-8/AHI AOD retrievals derived from (a) the
original DT and (b) the DTDL algorithms for the year 2017. Here, all matched pairs of
AHI retrievals and ground measurements are used. The diurnal variation derived from
ground-based measurements is shown in red, and the bias between AHI and ground
AODs is shown in grey. The shaded areas represent the standard deviations.



Fig. 8. Comparisons between AERONET AOD and AOD derived from the original DT method for (a) medium-quality and (b) high-quality data for the year 2017. Comparisons between AERONET AOD and AOD derived from the DTDL method for (c) medium-quality and (d) high-quality data for the year 2017. The dashed grey lines are plotted as Y=0.8X and Y=1.2X (positions of 20% error). The correlation coefficients (R), root-mean-square errors (RMSE), number of samples (N), and mean absolute errors (MAE) are given in each panel.

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Fig. 9. Comparisons between AERONET AOD and AOD derived from the original DT 1016 method for regions (a) R1, (b) R2, (c) L1, and (d) L2. Comparisons between AERONET 1017 1018 AOD and AOD derived from the DTDL algorithm for regions (e) R1, (f) R2, (g) L1, and (h) L2, with the training datasets obtained over regions (e) R2, (f) R1, (g) L2, and 1019 (h) L1. This process ensures independence of the validation datasets. The dashed grey 1020 1021 lines are plotted as Y=0.8X and Y=1.2X (positions of 20% error). The correlation coefficients (R), root-mean-square errors (RMSE), number of samples (N), and mean 1022 absolute errors (MAE) are given in each panel. 1023



Fig. 10. Absolute biases between AOD derived from ground measurements and retrieved from AHI in 2017 for different (a) $SR_{0.47}$, (b) $SR_{0.64}$, (c) $NDVI_{SWIR}$, and (d) scattering angles. The original DT (red lines) and DTDL (blue lines) algorithms are used. The shaded areas indicate standard deviations. The grey bars represent the frequency of occurrence of these parameters.

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