LGHAP v2: A global gap-free aerosol optical depth and PM_{2.5} concentration dataset since 2000 derived via big <u>earth_Earth_</u>data analytics

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Abstract. The Long-term Gap-free High-resolution Air Pollutants concentration dataset (LGHAP) generated in our previous study provides provides spatially contiguous daily aerosol optical depth (AOD) and fine particulate matters (PM2.5PMs) concentration-data-s at a 1-km grid resolution in China since 2000. This advancement empowered some-unprecedented assessments of regional aerosol variations and its their its influence impacts on the the environment, health, and climate overim the past few-twenty yearsyears. However, there is a need to improve enhance such a MODIS-like gap free high resolution quality AOD and PM2.5 concentration dataset with new robust features and extended spatial coverage. In this study, we present the version 2 of such a global-scale LGHAP dataset (LGHAP v2), which that was generated using an improved big earthEarth data analytics approach-via a seamless integration of distinct-versatile data science, pattern recognition, and deep-machine learning methods. Specifically, To better reconstruct the global AOD distribution from daily remotely sensed MODIS AOD imageries, multimodal AODs and air quality measurements acquired from relevant satellites, ground monitoring stations, and numerical models across the globe throughout the past two decades were firstly harmonized by harnessing the capability of random forest-based data-driven models. ThenSubsequently, an improved tensor-flow-based AOD reconstruction algorithm was developed to weave the harmonized multi-source AODs products together for gap_-filling data gaps in Multi-Angle Implementation of Atmospheric Correction (MAIAC) AOD retrievals from Terra. The results of the ablation experiments demonstrated better performance of the improved tensor-flow-based gap-filling method has a better performance in terms of both convergence speed and data accuracy. Ground-based validation results indicated a good data accuracy of the this global gap-filled free AOD dataset, with a site specific correlation coefficient (R) R of 0.85 and root mean square error (RMSE)RMSE of 0.14 compared toagainst the worldwide AOD observations from AERONET, which is better than outperformeding the purely reconstructed AODs (R = 0.83, RMSE = 0.15) and whereas slightly worse than the raw-raw Multi-Angle Implementation of Atmospheric Correction (MAIAC) AOD retrievals from Terra (R = 0.88, RMSE = 0.11). RegardingFor PM2.5 concentration mapping, aA novel deep-learning model approach, termed as the scene-aware ensemble learning graph attention network (SCAGAT), was developed hereby applied to enhance the estimation accuracy of global_better predict PM2.5-concentrations across the globethrough gap free AOD data. WhileBy gaining a better ByWhile enhancing accounting for the spatial scene representativeness of data-driven models across regions, the SCAGAT algorithm performed better superiorly inbetter during spatial extrapolation, largely reducing modeling biases over regions with limited

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and/or even absent even though the in situ PM_{2.5} concentration measurements are limited or absent. The sSite specific validation results indicated that the gap-free PM_{2.5} concentration estimates exhibit higher prediction accuracies, with an R of 0.95 and an RMSE of 5.7 µg m⁻³, compared togainst the PM_{2.5} concentration measurements obtained from previouspriorly heldhold-out sites worldwide. Overall, while while leveraging state-of-the-art methods in data science and artificial intelligence, a quality enhanced quality enhanced LGHAP v2 dataset was generated through big Eearth data analytics by cohesively weaving together multimodal AODs and air quality measurements from different diverse sources together cohesively. The gap-free, high-resolution, and global coverage merits render the LGHAP v2 dataset an invaluable data-base to advance aerosol-and haze-related studies and, as well as to trigger multidisciplinary applications for environmental management, health—risk assessment, and climate change analysisattribution. All gap-free AOD and PM_{2.5} concentration grids in the LGHAP v2 dataset, as well as the data user guide and relevant visualization codes, are shared online publicly accessible at https://zenodo.org/communities/ccnu_lghap (Bai et al., 2023a)₂₅ with a_data user guide and relevant visualization eodes available at https://doi.org/10.5281/zenodo.10216396.

1. Introduction

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Atmospheric aerosols, <u>produced from</u> either natural or anthropogenic <u>emissions</u>, have been proven to pose significant threats to human health, ambient environment, and climate (Up in the aerosol, 2022). The risks to public health from aerosol pollution are <u>elearevident</u>, with about 4.2 million deaths per year attributable to the exposure of fine aerosol particles, as stated by the World Health Organization (WHO, 2022). With increased aerosol loading, aerosols can significantly impair atmospheric visibility <u>because ofdue to</u> the hygroscopic effect, thereby reducing direct solar radiation on the Earth's surface (Liu et al., 2020; Wang and Yang, 2014; Wild et al., 2021; Yang et al., 2016). In addition to <u>the</u> evident <u>influenceimpaets</u> on air quality (Li et al., 2017), atmospheric aerosols also have an important and complex influence on regional, and even global climate (Anon, 2022; Guo et al., 2016, 2019; Li et al., 2019; Yang et al., 2020; Zhao et al., 2020). Therefore, an accurate monitoring of <u>the</u> atmospheric aerosol loading is vital for improving our understanding of <u>the</u> human-driven ambient environment and exposure pathways in health—-risk assessment.

Aerosol optical depth (AOD), a measure of aerosols distributed within an air column from the Earth's surface to the top of the atmosphere, has been widely used as a key indicator of total atmospheric aerosol loading. AOD observations from ground monitoring stations have long been recognized as the ground truth, and a few <u>gG</u>round-based aerosol observing networks, <u>e.g.such as</u>, the internationally collaborated Aerosol Robotic Network (AERONET), China Aerosol Remote Sensing Network (CARSNET), and Sun=_Sky Radiometer Observation Network (SONET), <u>were_had_been_established_to_provide global and/or regional aerosol measurements-have long served as the ground truth for AOD monitoring (Che et al., 2015; Giles et al., 2019; Li et al., 2018). However, the sparse distribution of <u>ground_aerosol</u> monitoring stations poseposes as significant challenges <u>into</u> gaining a <u>better-comprehensive</u> understanding of <u>the</u> aerosol variations across the globe.</u>

Satellite-based AOD products data well bridge thissuch a gap by providing spatially resolvedspatially resolved AOD retrievals with a vastextensive spatial coverage. Over the past forty years, A-a variety of space-borne instruments, e.g., Sea-<u>V</u>viewing Wide Field-of-<u>V</u>view Sensor (SeaWiFS), Moderate Resolution Imaging Spectroradiometer (MODIS), Visible Infrared Imaging Radiometer Suite (VIIRS), and Polarization and Directionality of the Earth².²¹/₋'s Reflectances (POLDER), werehad been deployed onboard different various satellite platforms and launched into space over the past forty_years (Wei et al., 2020). These versatile instruments provide ample AOD and aerosol property measurements, enabling us to map global AOD distribution with finer spatial resolutions in a long run. Nonetheless, satellite-basedsatellite-based AOD retrievals often suffer from excessive data gaps because of due to extensive cloud covers and retrieval failures^{3,57} significantly impairing the data application potential, of these spatially incomplete AOD imageries. Moreover, substantial data gaps in satellite-based AOD products could <u>as well as and resulting</u> in large uncertainties when assessing <u>the influence of aerosol impacts</u> on weather and climate.

A variety of gap-filling methods were developed and applied to reconstruct <u>the</u> missing values in <u>the</u> satellite remotely sensed <u>satellite</u> AOD images (Wei et al., 2020; Xiao et al., 2021). The simplest method is to fill in data gaps with valid observations from <u>other-alternative</u> data sources, e.g., filling in data gaps in MODIS AOD images from Terra with AOD observations from Aqua (Bai et al., 2019; Sogacheva et al., 2020); or <u>simply to</u> fusinge with AOD simulation outputs from numerical models (Xiao et al., 2021). Such a substitution method is straightforward and effective, <u>particularlyespecially</u> in an era with big <u>Fearth</u> observation data. Nonetheless, cross-mission biases <u>are always salient among between</u> satellite-based retrievals; <u>stemmingacquired from different various platforms and/or instruments</u>, are always salient because of the<u>due to</u> significant differences in <u>both</u>-instruments <u>properties</u> and<u>or</u> retrieval algorithms. <u>Thus</u>, <u>b</u>Bias correction is <u>thus</u>-essential to reducing systematic biases (Bai et al., 2016b, 2016a); <u>and and dDistinctifferent</u>-methods; such as linear regression and maximum likelihood estimation; <u>were are often</u> applied to account for<u>address</u> cross mission biases prior tobefore merging the datafor this purpose merging (Bai et al., 2016a, 2016b, 2019; Ma et al., 2016; Xu et al., 2015). More complex <u>data fusion</u> methods, like the Bayesian maximum entropy-(<u>Tang et al., 2016; Wei et al., 2021b</u>).

Another type of gap-filling methods works, in a-principle, to recover missing information via dominant pattern recognition and reconstruction over space and time, and the data-Data interpolating_INterpolating_empirical_Empirical_orthogonal Orthogonal functions-Functions (DINEOF) method is a representative one (Beckers and Rixen, 2003; Liu and Wang, 2019). Two similar methods were developed to fill-_in-data gaps in the ground-measured PM2.5 concentration time series and geostationary satellite-sensed AOD imageries (Bai et al., 2020; Li et al., 2022b). Similarly, Zhang et al. (2022) developed a spatiotemporal fitting algorithm to gap-fillfill gaps in the daily MODIS AOD product, primarily by predicting, with-AOD values mainly predicted based on annual trends and spatial residues inferred from neighboring pixels. Nonetheless, filling data gaps are hardly to be properly reconstructed simply based on with a single data source_is always challenging, particularlyespecially for those with excessive_extensive missing values (e.g., satellite-based AOD). Retrieving the missing AOD informationLeveragingLearning missing values from diversecternal from diversified external data productsinformation, via various_artificial_intelligence_learning algorithms, in artificial intelligence, such as e.g., numerical AOD simulations (Li et al., 2020; Xiao et al., 2017) and_even-meteorological factors (Bi et al., 2019), was proven to be-an effective and feasible way tofor improve theing spatial coverage of reconstructed AOD fields.

Given the powerful approximation capacity, the mMachine_learning method is anothers have been widely applied used approach forto downsealinge and bias-correcting numerical AOD simulations to match satellite AOD footprints, while data gaps in satellite based AOD imageries were then filled with downscaled data (He et al., 2023; Wei et al., 2021a); Given the powerful approximation capacity, machine_learning methods were extensively used for bias correction in gap filling problems over recent years (Bai et al., 2022b, 2023b; He et al., 2023; Wang et al., 2022; Wei et al., 2021a; Xiao et al., 2021). MLeveraging machine_learning and tTensor_completionflow-based methods, i.e., a more complex big data analytics framework, wereaswas developed useddeveloped to integrateintegrate six satellite-based AOD datasets and numerical aerosol diagnostics, as well asand in situ air quality measurements (Bai et al., 2022a), while a machine-learning method, i.e., random forest, was applied for downscaling and bias-correction purposes (Bai et al., 2022a). Based onHarnessing multimodal data fusion and missing value reconstruction capabilities this data analytics approach, a long-term gap-free high-resolution MODISlike AOD and PM concentration_dataset (LGHAP version 1), was successfully vielded generated overin China, withThe comparable an overall data accuracy comparable of reconstructed AODs well demonstrate the efficacy of thisto raw satellite retrievals, from which gap-free PM_{2.5} and PM₁₀ concentrations were mapped on a daily basis-gap filling approach, vielding a long-term gap-free high-resolution MODIS-like AOD and PM concentration dataset (LGHAP version 1) in China. Despite the good performance, _Despite the good reconstruction performanceadditionalRecent, additionalfurther investigations have recently recently proven that the critical importance of prior information is vital forinon tensor-flow-based gap-filling procedure, particularlyespecially over areas with substantial missing values, and the reconstruction results would be prone to significant_large uncertainty with few valid observations in the input tensor (Bai et al., 2022a; Li et al., 2022a, 2022b). Moreover, the strategies of maintaining an invariant background filed and assigning equal weights for to different AOD inputs may not only reduceslow down the convergence speed andbut degrade the reconstruction accuracy.

In this study, we present AnLeveraging an improved big Eearth data analytics approach has generated , a new global scale LGHAP dataset, referred to as termed as LGHAP v2 hereafter, hereafter, was hereby generated towhich furnishesextends provide daily global gap-free AOD and PM_{2.5} concentrations from China to worldwide at a 1-km grid resolution as ofdating back to for the period of 2000 to 2021. Toln order to accommodate massive global massive Eearth observations acquired from diverse satellites, numerical models, and air quality monitoring stations sources, an improved big Earth data analytics approach was developed by harnessing several new algorithmic improvements were applied to enhance the tensor-flow-based AOD gap filling approach. These improvements, includeing an attention reinforced tensor construction strategy and, an adaptive background information updating scheme, an optimized global data tile partition and rank updating, all aimeding at improving convergence speed and mitigating modeling bias propagation in numerical reconstructed AOD diagnosticsfields. Moreover, a novel deep-learning method -, namely, named as the SCene-Aware ensemble learning Graph ATtention network (SCAGAT), ----, --was developed applied to fulfill far-more accurate global PM2.5 concentration mapping across the globe, particularly over regions with limited air quality monitoring stations. While bBBenefiting from the customized algorithmic improvements and the novel-innovative_SCAGAT PM2.5 concentration mapping methodapproach, the LGHAP v2 dataset has not only has an not only extended the spatial coverage from China to worldwideglobal scaleworldwide, global boasting and but also but also - improved data accuracy-compared to LGHAP v1. To our knowledge, this is the first publicly accessible and global long term gap free MODIS like AOD and PM2.5 concentration dataset with a daily 1-km resolution, which could be used to help deepen our understanding of global aerosol pollution variations as well as adverse impacts on public health and on the, ecosystem, weather, and climate. In the following sections 2 and 3, we provide provide ed a more detailed<u>comprehensive</u> description of <u>the</u> diversified data sources analyzed in this study, as well as <u>the versatile artificial</u> intelligent machine-learning and deep-learning methods used to manipulate big Eearth observational data. In the subsequent sections 4 and 5, tThe pPerformance of algorithmic improvements as well as, the data accuracy of the global gap free AOD and PM2.5 concentration data, and the application potential of the LGHAP v2 dataset data were then comprehensively evaluated. To our knowledge, As a the LGHAP v2 is the first-publicly accessible and global long-term gap-free MODIS-like AOD and PM_{2.5} concentration dataset, the LGHAP v2 servers as a promising data source to improve our understanding This resource stands to of global aerosol pollution dynamics, shedding light on and its their adverse impacts on public health, ecosystems, weather-patterns, and climate-change. by comparing it to against the worldwide in_situ AOD and PM2.5-concentration measurements

2. Data Sources

In the current<u>this studySimilar as our previous study</u>, here we still attempt aim to synergistically integrate the big Eearth data acquired from diverse sources to generate <u>a</u> global long-term gap-free AOD dataset with <u>a</u> daily 1-km resolution. <u>Subsequently</u>, from which, from which sepatially contiguous PM_{2.5} concentration estimates can be then derived usingby a more robust and accurate data-driven approach way to minimize the gaps and maximize the prediction accuracy. As shown in Table 1 <u>illustrates</u> array variety of big Eearth data were hereby employed in data production this study, including gridded AOD products from six polar orbiting satellites<u>ans</u>-numerically simulated MERRA-2 AOD and aerosol diagnostics, <u>eleven-ten</u> meteorological reanalysis fields, <u>and-six</u> datasets of in situ AOD and air pollutant<u>s</u> concentration<u>s</u> measurements. Additionally, auxiliary <u>variables-parameters</u> representing land use and land cover types, elevation, <u>and</u>-population density<u>s</u> as <u>well as <u>a</u>and-vegetation <u>indexcovers</u>, were <u>used not only to helpineorporatedalso</u> employed as critical explanatory variables to harmonize <u>the</u> discrepancies among <u>multimodal</u> heterogeneous <u>aerosol</u> data<u>sets</u> prior to data integration. Note the spatial and temporal resolution as well as the time period for each data product are different from that of the benchmark dataset, namely, the MAIAC AOD product, and a data homogenization method is therefore essential to account for such discrepancies to reduce possible bias propagation in the subsequent data fusion procedure. <u>and</u>but also to aid in <u>the</u> global PM_{2.5} concentration mapping.</u>

Table 1. Summary of the diverse big Earth data used in this study to help generate a-global gap-free AOD dataset and $PM_{2.5}$ concentrationsat a daily-<u>and</u> 1-km resolution (LGHAP v2) from 2000 to 2021.

Category	DatasetProduct	Temporal Resolution	Spatial Resolution	Time Period	
	MCD19A2 (MAIAC)	daily	1 km	2000-2021	
	Terra/MISR	daily	4.4 km	2000-2021	
	NPP/VIIRS	daily	5 km	2012-2021	
AOD	Envisat/AATSR	daily	10 km	2000-2012	
	PARASOL/POLDER	daily	10 km	2005-2013	
	SeaWiFS/OrbView-2	daily	10 km	2000-2010	
	AERONET	hourly	<u>N/A</u>	2000-2021	
	Air temperature	hourly			
	U/V component of wind	hourly			
	Relative humidity	hourly			
	Surface pressure	hourly			
Meteorological	Boundary layer height	hourly	0.25°	2000-2021	
factors	Total column water vapor	hourly			
	Surface solar radiation downwards	hourly			
	Total precipitation	hourly			
	Instantaneous moisture flux	hourly			
	Visibility	3-hour	<u>N/A</u>	2000-2021	
Air quality measurements	PM _{2.5} , PM ₁₀ , NO ₂ , SO ₂ , CO	hourly	<u>N/A</u>	2000–2021	
Population	WorldPop	annual	1 km	2000-2020	
Land cover	Impervious (GISA)	annual	30 m	2000–2020	
	MCD12Q1	annual	500 m	2000-2021	
NDVI	MOD13A3	monthly	1 km	2000-2021	
Aerosol diagnostics	MERRA-2	hourly	$0.5^\circ imes 0.625^\circ$	2000-2021	
Elevation	SRTM DEM	<u>N/A</u>	90 m	<u>N/A</u>	

2.1. Satellite-<u>Bb</u>based AOD <u>Pp</u>roducts

The_AOD retrievals_ derived from MODIS_sensor observations-on board Terra (AODTerra) with-using_the Multi-Angle Implementation of Atmospheric Correction (MAIAC) algorithm_(denoted as AODTerra afterwards), were_hereby usedservedwere hereby used as the benchmark to-for generatinge the global long-term gap-free AOD dataset, given their finer spatiotemporal resolution and longer temporal coverage (Lyapustin et al., 2011, 2018; Mhawish et al., 2019). Previous studies have demonstrated the a bettersuperior quality of the <u>AODTerra</u> MAIAC AOD data relative to other gridded <u>AOD</u> products (Chen et al., 2021; Martins et al., 2017; Qin et al., 2021)-and in regard to, not only data accuracy andbut also spatiotemporal completeness, even better than those retrieved with the well-known Dark Target and Deep Blue algorithms (Jiang et al., 2023; Liu et al., 2019). Figure S1 presents the spatial and temporal distribution of the coverage ratio of valid AOD_{Terra} from 2000 to 2021 at each satellite footprint across the globe.

Satellite-based AOD retrievals from a few key instruments other than MODIS were <u>also</u> applied to support gap filling of AOD_{Terra} and- tThey include: (1) <u>Visible Infrared Imaging Radiometer Suite</u> (VIIRS₇ on board Suomi-NPP), (2) Multi-<u>Aaa</u>ngle Imaging SpectroRadiometer (MISR, on board Terra), (3) Advanced Along-Track Scanning Radiometer (AATSR, on board Envisat), (4) <u>POLarization and Directionality of the Earth's Reflectance</u> (POLDER₇ on board PARASOL), and (5) <u>Sea-Viewing Wide Field of View Sensor</u> (SeaWIFS₇ on board SeaStar). Meanwhile, MAIAC AOD data from MODIS on board Aqua were also applied as the <u>an important</u> complementary data-<u>set_source-to support gap filling of AOD_{Terra}. Given their varied the different</u> overpassing times and temporal spans, these multisensory AOD <u>dataset_canproducts</u> provide complementary observations to help reduce random errors when <u>during the AOD data</u> reconstruction <u>ofng data gaps in AOD_{Terra}procedure because ofdue to</u> the <u>known increased</u> prior knowledge. <u>A brief summaryMore details</u> of these AOD products <u>datasetsproducts</u> can be found in Bai et al. (2022a) and Wei et al. (2020).

2.2. Ground-<u>Bb</u>based AOD Observations and Arir Oquality Mmeasurements

2.2.1. AERONET AOD Oobservations

Ground-based AOD observations from AERONET have long been used as the ground truth to-for_validatinge AOD retrievals from other instruments, <u>particularlyespecially diverse</u> satellite-based AOD retrievals. In this study, AOD observations from AERONET (across the globe) during the study period were employed as an independent data source to validate the data accuracy of the global gap-filled AOD dataset. To guarantee an adequate number of AERONET AOD samples, the Level 1.5 (instead of rather than Level 2.0) AOD observations instead of Level 2.0 were applied, though the latter has stricter screening criteria for quality control. For spatial registration, each AERONET AOD observation was spatially collocated with mean AOD values over grids within a 50×50 km window size. Figure S2 presents the spatial distribution of the AERONET sites and the air quality monitoring stations that provide ing the pivotal AOD and PM_{2.5}-concentration observations-used in this study.

2.2.2. Air **Qquality** <u>Mmeasurements</u>

Concentrations of PM_{2.5} and other relevant air pollutants, like NO₂, SO₂, PM₁₀, and CO₂ were acquired from a few <u>environmental</u> agencies and/or monitoring centers, such as the United States Environmental Protection Agency, European Air Quality Portal, China National Environmental Monitoring Centre, Canada National Air Pollution Surveillance, and Japan National Institute for Environmental Studies, to name a few. Moreover, air quality measurements acquired from the World's Air Pollution Index, an open-source data hub, were included as well. <u>To guarantee uniformity and comparability of these ground-based data, we conducted necessaryGiven potential differences in measuring principles and quality control criteria, preprocessing towe performed rigorous data cleaning measures to standardizeharmonize these multisource air quality</u>

measurements, as well as including not only the removal of outliers but also-converted the time-series to an unification of time scales to a daily average scale synchronized with satellite observations taken on the same dates. The PM2.5 concentrations were used as the learning target for global PM2.5 concentration mapping. Aiming toat provideing critical prior-information to facilitate the AOD gap-filling, the ground-based air quality measurements were also used as an important proxy for regional in situ AOD prediction, benefitting from largely because of the relatively dense distribution of air quality monitoring networks as well as and exploited the good-associations between aerosol loadings and regional air pollutants concentrations.

Atmospheric visibility, a common air quality indicator-that is highly associated with aerosol loadings, <u>waswere</u> acquired from worldwide meteorological monitoring stations and used <u>as the critical predictor</u> <u>likesimilar to air pollutants</u> <u>concentrations</u> to predict AOD over each monitoring site via data-driven modeling. Given <u>the much denser distribution of</u> ambient air quality and meteorological monitoring sites, as shown in Figure S2, for the spatial distribution of global air quality and meteorological monitoring sites, as well as the good accuracy of site based AOD predictions (Bai et al., 2022b; Li et al., 2022b), a global virtual AOD monitoring network was <u>in turn</u> established, <u>harnessing the associations between</u> <u>AOD and air quality relevant parameters.</u>, <u>ThisSuch a virtual network providesing</u> us with an unparalleled opportunity to improve AOD gap-filling accuracy and efficiency, <u>particularly especially for inover</u> regions <u>being disturbed by with</u> massive data voids in satellite AOD data voidsimageries-(Bai et al., 2022b; Li et al., 2022b).

2.3. Numerical Ssimulations

2.3.1. MERRA-2 Aaerosol Ddiagnostics

Despite the coarse spatial resolution and large modeling bias, tThe Modern-Era Retrospective Analysis for Research and Applications, version 2 (MERRA-2) aerosol diagnostics, including total AOD and ehemical-aerosol components like black carbon, organic carbon, dust, and sulfate aerosols, were employed to provide prior information to advance AOD gap-filling. As the-NASA's latest reanalysis for the satellite era, MERRA-2 is generated using the newly Earth system model, of Goddard Earth Observing System, version 5 (GEOS-5), providing global simulations of a variety of geophysical and chemical variables on the Earth's surface. More detailsed descriptions of the assimilation system and the data quality of MERRA-2 aerosol reanalysis can be found in the literature, such as Buchard et al. (2017) and Randles et al. (2017). By taking AOD_{Terra} into account as a the learning target, data-driven models were established to <u>spatially</u> downscale and bias-correct MERRA-2 AOD background-field to the level of AOD_{Terra}, with with MERRA-2 aerosol diagnostics as well as meteorological, geographical, and socioeconomic factors-used used as covariates. This The downscaling model not only improves the spatial resolution andbut also corrects large modeling biases in MERRA-2 AOD. Given the global complete coverage merit, downscaled and bias-corrected MERRA-2 AOD background-field, given its spatially contiguous coverage, the downscaled gap free AOD data wereas then used as critical prior information to facilitate the AOD gap-filling of AOD_{Terra}, in particularly over regions lacking observational AOD.

2.3.2. ERA-5 <u>R</u>reanalysis

As the latest atmospheric reanalysis produced by the European Center for Medium Weather Forecast, ERA-5 provides hourly estimates of a variety of atmospheric, terrestrial, oceanic, climatic, and meteorological variables. The data are provided for <u>a at about</u> 30 km grid resolution on the Earth's surface, resolvingdelineating the atmosphere layer using 137 levels from the surface up to a height of 80 km, covering the period from January 1940 to the present (Hersbach et al., 2020). Atmospheric parameters, including surface pressure, air temperature, relative humidity, wind speed, total column water, total precipitation, surface solar radiation downward, instantaneous moisture flux, and boundary layer height, were retrieved acquired from ERA-5 and used as important modeling covariates, not only in both data harmonization models_and_to calibrate other AOD and

relevant data products to the level of AOD_{Terra}, but also <u>and</u>, in <u>global</u> PM_{2.5} mapping model<u>ss</u>, to help approximate nonlinear associations between PM_{2.5} and AOD. <u>A simple b</u>Bilinear interpolation was applied to <u>the map</u> ERA-5 reanalysis data down to <u>convert them to</u> the AOD_{Terra} footprint resolution for spatial registration.

2.4. Auxiliary Delata

Several socioeconomic and geographic factors were also applied as covariates to support predictions of AOD gap filling and PM_{2.5} concentration predictionsmapping. Specifically, gGridded population data from WorldPop were used to indicate the spatial distribution of residents, which were appliedserving as a critical proxy offor anthropogenic aerosol pollutionair pollutants emission intensity. To resolve characterize the land--use-dependent aerosol emissions, land cover types and the vegetation index derived from MODIS- retrieval observations-products, along withas well as the coverage ratio of the impervious surface calculated at the AOD_{Terra} footprintfrom the land use dataset generated by Huang et al. (2022),-were also applied. The dDigital elevation data collected from the Shuttle Radar Topography Mission (SRTM) with a resolution of 1 arcsecond were used to characterize the potential impacts of topography on aerosol loadings.

3. Methods

3.1. Tensor-Fflow-based AOD Rreconstruction

3.1.1. Overview of AOD Ggap-Ffilling Mmethod

Deriving spatially contiguous PM_{2.5} concentrations from gap-filled AOD images has been-proven more promising for a better spatial analysis of large-scale PM_{2.5} distribution (Bai et al., 2022b). In this study, the big <u>E</u>earth data analytics <u>framework</u> proposed in Bai et al. (2022a) was further adapted <u>and improved</u> for generating global gap-free AOD imageries to support various content-based mapping. <u>As shown in</u> Figure 1, presents the workflow of the improved <u>big Earth data analytics</u> framework of the big <u>E</u>earth data analytics for generating global gap filled MODIS like AOD maps. This framework-<u>also</u> consists of three primary data manipulation procedures, including: 1) machine_-learned multimodal data homogenization, 2) knowledge-reinforced AOD tensor compiling, and 3) tensor-flow-based AOD reconstruction, with algorithmic improvements primarily conducted in the latter two procedures. This improved big <u>E</u>earth data analytics approach empowered us to weave together multimodal AODs and versatile big <u>E</u>earth observations from diversified diverse sources, together neatly via a synergy of state-of-the-art machine_ learning and tensor completion methods. <u>Because-Since</u> the technical flow of this big <u>E</u>earth data analytics framework was <u>elaboratedpreviously detailed-on well elaborated</u> in Bai et al. (2022b), we <u>hereby</u> only provided an overview of this method while emphasizing the newlydescribing more details of the newly developed algorithmic components in the following subsections.

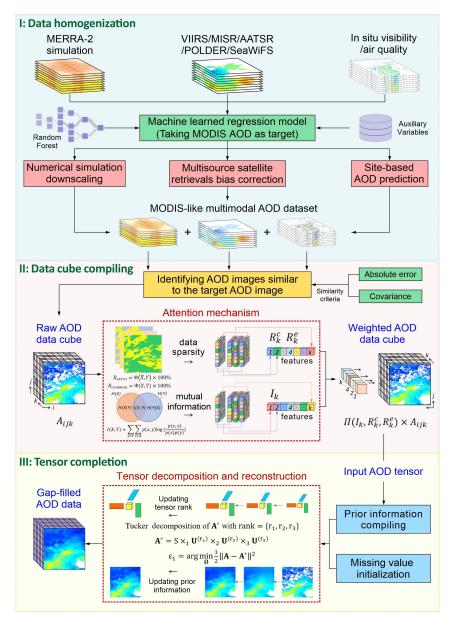


Figure 1. A schematic illustration of the enhanced-improved big earthEarth data analytics for generating the MODIS-like global gap-free AOD dataset.

The overall architecture of this big Earth data analytics framework was summarized as follows. MRLeveraging random forest based regression models, multimodal AODs₁ and relevant aerosol data acquired from different satellites, ground monitoring stations, and numerical models were firstly harmonized to resemble the baseline dataset of AOD_from Terra retrievals (AOD_terra) terra, aiming to at not only minimizeing both cross-sensor biases arising from algorithmic differences and spatial heterogeneities and to but also accounting for spatial heterogeneities because of due to different spatial resolutions. This Theis data homogenization process is vital for the tensor-flow-based AOD gap-filling, because the bias-corrected and downscaled AOD estimates were critical inputs to form the AOD data cube. More details related to the multisource data homogenization were described in Text S1 in the supporting information. The AOD data cube was then created based on homogenized data at each individual data tile. A proper AOD data cube compiling is undoubtedly essential for the tensorflow based AOD reconstruction. To fill data gaps in each individual AOD_{Terra} image, an AOD data on the same date, along with historical AOD_{Terra} images resembling similar spatial patterns over the same region. Because of the Due to excessive nonrandom missing values in the AOD_{Terra} imageries, both the downscaled MERRA-2 AOD grids and AOD estimates derived from air quality and visibility measurements were used conjunctively to identify <u>the historical similar AOD_{Terra}</u> imageries with a <u>similar spatial distribution</u> from the historical image series. The selected historical AOD_{Terra} images and <u>bias-corrected</u> <u>bias</u> <u>corrected</u> AOD images from other satellites on the same date were <u>used</u> individually <u>incorporated</u> as a slice of the tensor. Additionally, dispersed in situ AOD estimates and 5% <u>of the</u> randomly selected AOD estimates from the downscaled MERRA-<u>2 AOD</u> data were directly overlaid onto the corresponding AOD_{Terra} grids <u>where-without</u> valid <u>AOD</u> retrievals<u>were not</u> presentabsent. These implementations <u>not only</u> helped improve the gap-filling accuracy <u>andbut also greatly</u> boosted the convergence speed given the provision of prior knowledge.

High order singular value decomposition (HOSVD), an orthogonal Tucker decomposition method, was finally-applied to each well-compiled AOD data cube for tensor-flow-based pattern recognition and tensor data completion. Data gaps within the input AOD tensor were firstly filled with the spatial average of each individual AOD image to initializete the tensor decomposition. The AOD tensor was then decomposed along every each two-dimension of AOD tensorslice independently, and a new tensor was subsequently reconstructed based on the principal modes learned along every each two dimension slice of the tensor via a low-rank approximation (i.e., generating an approximating matrix with reduced rank for compression). During thise tensor reconstruction processprocedure, the AOD_{Terra} observations in the target image to be gap-filled were deemed as the hard data (i.e., true state and invariant throughout the tensor completion procedure) while multisensory AOD estimates and historical AOD_{Terra} images were usedserved as the soft data (prior supporting information and updated by iterates till convergence). By iteratively adjusting the dimension-varied ranks, the data values over grids to be gap-filled were updated and tuned to optimize both spatial homogeneity and information entropy concurrently (Bai et al., 2020, 2022a). This The tensor completion process continued till it reacheding an good agreement (with a bias decay ratio < 0.1%) between the reconstructed values and the previouslypriorly reserved AOD_{Terra} observations.

3.1.2. Algorithmic Limprovements

To accommodate <u>the</u> massive data analytics for global-scale AOD gap-filling, <u>two-three</u> major algorithmic enhancement modules were incorporated to help improve the reconstruction efficiency and accuracy, <u>foeusing-with particular focus</u> on <u>the</u> optimiz<u>ationing of</u> data manipulation procedures in tensor-flow-based AOD gap_filling. <u>Instead of</u>Rather than treating each slice of data in <u>the</u> raw AOD data cube equally, an attention mechanism was introduced to optimize the AOD tensor compiling, aiming at underscoring the importance of those AOD imageries with fewer data gaps while more closely resembling the target AOD_{Terra} imagery during tensor flow based AOD reconstruction. Meanwhile, an adaptive prior information updating scheme was implemented to help mitigate the propagation of large modeling<u>modelling</u> biases in numerical AOD diagnosties to the final reconstructed fields during the tensor reconstruction procedure. Moreover, the rank updating strategy was optimized to improve <u>the</u> computing efficiency in tensor completion.<u>A</u> The algorithm 1 below presents the pseudo code of the optimized algorithm used for tensor-flow-based AOD reconstruction.

Algorithm 1. The pseudo code of the optimized algorithm used for tensor-flow-based AOD reconstruction.

Input: tensor $\mathbf{A} \in \mathbf{R}^{N_1 \times N_2 \times N_3}$ with $\mathbf{\Omega} = \{(i, j, k): A_{iik} \text{ is observed}\}$, threshold T_1, T_2 **Output:** reconstructed entries $\mathbf{A}' = \mathbf{A}^*(:,:,k^t) \in \mathbf{R}^{N_1 \times N_2}$ 1: Attention mechanism: $\omega_k = \prod(MI_k, R_k^c, R_k^e)$ $(i, j, k) \in \Omega$ $(\omega_k \cdot A_{iik})$ 2: Initialize $A_{ijk}^* =$ <u>∑i∑</u>j A_{ijk} $(i, j, k) \notin \Omega$ 3: for $r_3 = \frac{1}{3}N_3$ to 1 step -2 do 4: $n_1 = n_2 = 0$ while $\varepsilon_1 > T_1$ or $(n_1 < \frac{1}{3}N_1 \text{ and } n_2 < \frac{1}{3}N_2)$ do 5: 6: $n_1 = n_1 + 1, \, n_2 = n_2 + 1$ $r_1 = \frac{n_1 N_1}{75}, r_2 = \frac{n_2 N_2}{75}$ 7: $\mathbf{A}^* = \text{HOSVD}(\mathbf{A}^*, \text{rank} = \{r_1, r_2, r_3\}):$ 8: $\mathbf{A}^* = \mathbf{S} \times_1 \mathbf{U}^{(\mathbf{r}_1)} \times_2 \mathbf{U}^{(\mathbf{r}_2)} \times_3 \mathbf{U}^{(\mathbf{r}_3)}$ 9: $\varepsilon_1 = \arg\min_{\mathbf{A}} \frac{1}{2} \|\mathbf{A} - \mathbf{A}^*\|^2$ 10: 11: $A^*_\Omega = A_\Omega$ 12: $\mathbf{A}_{\widetilde{\mathbf{\Omega}}}^* = \omega_1 \mathbf{A}_{\widetilde{\mathbf{\Omega}}}^* + \omega_2 \mathbf{A}_{\widetilde{\mathbf{\Omega}}}, \ \widetilde{\mathbf{\Omega}} \text{ denotes background location}$ 13: end while if $\arg \min_{1} \frac{1}{2} || \mathbf{A} - \mathbf{A}^* ||^2 < T_2$ then 14: 15: break; end if 16: 17: end for

3.1.2.1. Attention-<u>R</u>reinforced AOD <u>T</u>tensor <u>C</u>eonstruction

As a widely used technique in deep_learning regimes, the attention mechanism is a mimic of cognitive attention allowing the model to focus on specific parts of the input data, achieved by assigning higher weights to more crucial elements in ensemble learning. Regarding the tensor-flow-based AOD reconstruction task, the_data slices with a higher similarity to the target image and fewer data gaps are supposed to should play a more important roles be accorded more significances than those-less similar ones with extensive data gaps during tensor completion. Three statistical metrics, i.e., including mutual information (Shannon, 1948), spatial coverage ratio of common observations (R_{common}) between each soft data and hard data, and spatial coverage ratio of extra observations beyond common observations in soft data (R_{extra}), were calculated to determine the <u>overall</u> weight that should be assigned to each data slice of data in the input AOD tensor. Specifically, mutual information was applied to gaugecharacterize the mutual dependencye between the target image and each slice of soft data reference AOD images, while cCommon spatial coverage ratio was used to quantifyindicate the reliabilitydata amount for-of mutual information calculation, while and extra spatial coverage ratio indicates -was employed to depict additional information content that can be provided by reference AOD imagessoft data. Equations (1–3) provide Below gives the formulas to calculate these three statistical metrics.

$$MI(X,Y) = \sum_{y \in Y} \sum_{x \in X} p(x,y) \log\left(\frac{p(x,y)}{p(x)p(y)}\right)$$
(1)

$$R_{common} = \Phi(X, Y) \times 100\% \tag{2}$$

$$R_{extra} = \Phi(\tilde{X}, Y) \times 100\% \tag{3}$$

<u>Note that where</u> X and Y refer to common observations in soft and hard data, respectively. The \tilde{X} denotes extra observations in soft data.₂₂, p(x, y) is the joint probability mass function of X and Y, and while p(x) and p(y) are the marginal distribution mass function of X and Y-, respectively. Additionally, $\Phi(X, Y)$ is the spatial coverage ratio of the common observations, and $\Phi(\tilde{X}, Y)$ is the spatial coverage ratio of extra observations in the soft data. By multiplying these three normalized weights to the corresponding soft data, an attention-reinforced AOD tensor was constructed in turn, which was then used as the input data cube for tensor completion.

3.1.2.2. Adaptive Pprior Linformation Uupdating

To facilitate <u>the_AOD</u> gap-filling over regions with <u>abundant_substantial_</u>data gaps, in our previous method, <u>the_</u>5% random samples from the downscaled MERRA-2 AOD image (AOD_{M2} hereafter) on the same date were used as prior information and <u>directly placed_overlaid_directly</u> onto grids without observational AOD (i.e., AOD_{Terra} and site-based AOD estimates from air quality and visibility measurements). Although this <u>empowered_usenabled</u> to improve<u>d</u> the convergence speed during tensor completion, <u>the</u> spatial patterns of the reconstructed field over regions with excessive data gaps were more likely to resemble the distribution of AOD_{M2} givendue to because of the <u>fixedthese</u> <u>-unchanged 5% backgroundprior</u> <u>information-values in the target AOD image</u> equal weight of the soft and hard data. In other words, sparse observational AODs derived from air quality measurements played a relatively weak role in tensor completion when confronteding with AOD_{M22}. In <u>thissuch a</u> context, large modeling biases in AOD_{M2} might be introduced into the final <u>reconstructed_reconstruction</u> fields.

In this study, we introduced an adaptive prior information updating scheme to help mitigate potential bias propagation from AOD_{M2}problem. Differing from the strategy used in our previous method, tThe main principle is to force tThe AOD prior information in the input AOD tensor was also forced to update by iterationsvely throughout the tensor completion process, rather than maintaining them as invariant as AOD_{Terre}-observations throughout the tensor completion process. Specifically, random AOD_{M2} samples were only used to initiate initialize the tensor construction, while weighted averages of these prior information and the corresponding reconstructed values were then used as new prior information for the next iteration. Meanwhile, the weights assigned to the reconstructed fields were gradually increased by iteration till convergence. The ultimate goalgoal was to improve the contribution of reconstructed reconstruction fields learning from actual observations while reducing the influence of AOD_{M2} background field. Additionally, Tthe The ablation experiments also-demonstrated that such a scheme isthe effectiveness of this scheme in mitigating bias propagation from AOD_{M2}, largely improving the reconstruction performance over regions with limited observational data.

3.1.2.3. Optimized Gglobal Ddata Ttile Ppartition and Rrank Uupdating

Given <u>tThe</u> high spatial and temporalspatiotemporal resolution of AOD_{Terra} imageries presents a, performing global-scale AOD gap-filling isgreat-thus_-challenging_challenge in performing global-scale AOD gap-filling because of the due to huge

computational burdens. To improve the computational efficiency and to make the computing workload manageable, the following algorithmic improvements adjustments were applied implemented. Firstly, the continental global AOD_{Terra} data over land<u>mass</u> were worldwide were divided into 480 data tiles, with AOD gap-filling performed over each data tile independently. The size of a tile was determined empirically after performingThrough a set of gap-filling trials with different-varying tile sizes, and a nominal tile size of a tile covering 700_×_700 pixels, refer to Figure S3 for the spatial distribution of the optimized data tiles, (could be different over coastal regions) was finally applied to balance the computing workload and reconstruction the learning accuracy. Figure S3 presents the spatial distribution of the optimized data tiles used in this study for global AOD gap-filling. Moreover, a 50-pixel overlap on the boundary of each tile was enforced, and an inverse distance weighting scheme was finally applied to these overlapped pixels_-when mosaicking the gap-filled tiles, aiming to eliminate the boundary effects between tiles toward a smooth distribution of AOD across the globe.

An optimized rank updating strategy was also proposed to improve the learning efficiency. In <u>the</u> tensor completion process, <u>Since the</u> tensor's decomposition and reconstruction processes in the tensor completion are driven by iteratively updating updated tensor ranks..., <u>aAn optimized rank updating strategy was also</u> hereby proposed to improve the learning efficiency. To improve the computational efficiency of global AOD gap-filling, we developed an optimized strategy to update the ranks between iterations. Specifically, the ranks were updated in an ascending order along with the first and second dimensions in the inner loops to enhance the spatial details of reconstructed AOD fields. In contrast, the ranks were updated in a descending fashion along with the third dimension in the outer loop to aggregate the target AOD_{Terra} image with the soft data in a low-rank approximation manner. This new rank updating strategy not only helps better resolve spatial details of AOD but also accelerate the convergence speed of tensor completion.

3.2. Global PM2.5 Ceoncentration modeling Modeling

The sparse and uneven distribution of ground-based air quality monitoring stations poses significant challenges to global PM_{2.5} concentration mapping, <u>particularlyespecially</u> over regions of with fewer PM_{2.5} concentration measurements (e.g., Africa and <u>S</u>south America in Figure S2). <u>AdditionallySoNonetheless,Also</u>, how to reinforce the <u>scene</u>spatial representativeness of data-driven models <u>when_to improve the spatial extrapolating-extrapolation accuracy them_overacross_extensive_spatial domainsee-is still elusive</u>. As a novel ideaIn this study, a recently developed deep learning method, namely, the <u>scene-aware ensemble learning graph attention network (SCAGAT)</u>, was hereby <u>developed and applied</u> to better estimate global PM_{2.5} concentrations from gap-filled AOD imageries by accounting for <u>the spatial scene</u>-representativeness of each data driven model. Instead ofRather than establishing a <u>single global PM_{2.5} estimation models were firstly developed using <u>method</u> representation measurements.</u>

For a given grid, raw PM_{2.5} concentration estimates were then-estimated from a set of independent site-specific PM_{2.5} estimation models₂, of which should resemble similar geographic scene features as the given grid cell_____under the assumption that the relationship between AOD and PM_{2.5} is similar over regions with an analogue environmental background. Nine distinct factors covering geodetic-geographic location, land cover types, climate zones, AOD levels, and population density were utilized to characterize the scene attributes of each grid cell. Subsequently, a graph attention network was used to aggregate these-raw PM_{2.5} concentration estimates derived from site-specific models to better predict the produce an ensemble PM_{2.5} concentration estimate grid cell₂. In the graph network, Wwith-weights assigned to the adjacency matrix were determined in reference to the differences between nine different scene features, and the node bias was given as the testing accuracy of each site-specific PM_{2.5} prediction model. Figure S4 presents depicts the workflow of the proposed SCAGAT model for global PM_{2.5} concentration mapping. This novel-innovative ensemble learning method enables us to better predict

PM_{2.5} concentrations across the globe, <u>particularly especially</u> over regions with <u>few_limited_or</u> even none in situ PM_{2.5} concentration measurements. <u>Figure S4 depicts the workflow of the proposed SCAGAT model</u>, and <u>aAdditionalMore</u> details <u>regarding of the SCAGAT model</u> were introduced in Text S2-as part of the supplementary information. For more detailed descriptions of this method, please refer to Li et al. (2024).

4. -Results

4.1. Efficacy <u>A</u>assessment of <u>A</u>algorithmic <u>E</u>enhancement <u>M</u>modules

Ablation experiments were firstly conducted to evaluate the accuracy improvement potential of each newly developed algorithmic enhancement module. Three case studies were simulated by masking actual AOD_{Terrn} retrievals with randomly selected cloud masks on different dates, and <u>the</u> methods reinforced with different enhancement modules were then applied to reconstruct <u>the previouslypriorly</u> holdout AOD values. For inter-comparison, the AOD gap-filling framework developed in Bai et al. (2022a) was used as the benchmark method. As shown in Figure 2, <u>the</u>AOD distributions <u>reconstructed were</u> reconstructed withusing-<u>a</u> methodsmethods embedding attention mechanism and adaptive background information updating modules have smaller bias levels compared to than the benchmark method, which in turn justify the efficacy of these two new algorithmic enhancement modules. Given an equal weight of each slice of data in the input AOD tensor, the reconstructed data fields from the benchmark method were prone to resembling a mean state determined largely by the principal mode of the input tensor. In this context, peak <u>and/or low</u> values in the target image might be underestimated (or overestimated for low values) if because of relatively few soft data resembling similar patterns in the input tensor (e.g., Figure 2c).

With the involvement of theBy incorporating the attention mechanism, each slice of data in the raw AOD data cube was adaptively weighted adaptively, with larger greater weights given to data slicesthose not only having larger broader spatial coverage and but also closer with similarities to the target AOD_{Terra} image. This strategy is vital to reducing contributions from irrelevant data, particularly especially when facing encountering with imunbalanced data samples in-within the raw AOD data cube, i.e., more irrelevant data and fewer similar imageries. Moreover, the importance of the target image was maximized during the tensor completion procedure by giving assigning it a 100% weight. Compared to the benchmark method, peak and/or lowextreme values in raw AOD_{Terra} images were better reconstructed using by the method embedding the attention mechanism. For instance, in Figure 2b, the benchmark method apparently overestimated low AOD values in the north, in Figure 2b were apparently overestimated by the benchmark method, whereas such an effect a discrepancy was largely mitigated using methods involving the attention mechanism.

In contrast to the benchmark <u>method by using which used an invariant background throughout the tensor completion process</u>, an adaptive background updating scheme was thus applied incorporated here to not only accelerate the convergence speed <u>andbut also</u> mitigate possible error propagation <u>arising</u> from numerical simulations to the final reconstructed reconstruction fields. Compared to the benchmark method, aAs illustrated in Figure S5, the enhanced method, involving adaptive background updating module, indicated enabled to superior detection and resolution offreduce the adverse impact of manually added outliers in raw background fields, compared to the benchmark. compared to the benchmark, the manually added outliers in raw background fields were better detected and reconciled by the improved method owing to the involvement of the adaptive background updating module, thusereby avoiding large error propagation from background fields into the reconstructed AOD data. Although tThe better quality of the reconstructed fields derived from the improved methods well demonstrates the efficacy of these two enhancement modules werecould be largely cancelled when dealing confronteding with images with containing excessive data gaps (e.g., Figure 2c,), showing only a marginal improvement in accuracy improvement

relative<u>compared</u> to the benchmark method. The inherent reason could be attribut<u>edable</u> to few observational data in the target image for reference to leverage <u>the</u> attention mechanism to pinpoint similar AOD images from the historical data series.

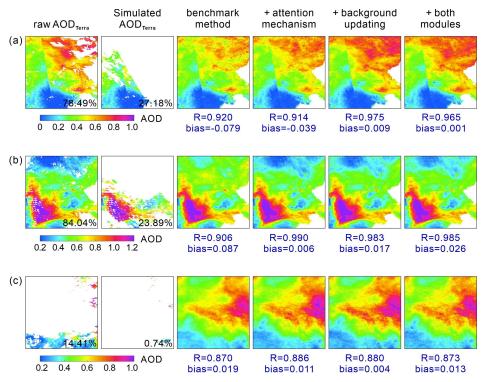


Figure 2. Performance evaluation of different algorithmic enhancement modules on the reconstructed AOD distribution. Raw AOD_{Terra} denotes <u>the</u> actual AOD retrievals from Terra, while simulated AOD_{Terra} refers to partially masked AOD_{Terra} . The benchmark method is the AOD gap-filling approach proposed in Bai et al. (2022a). The latter three columns present the reconstructed fields using the enhanced benchmark methods. The R and bias denote correlation coefficient and deviations between <u>the withheldholdout</u> observed and reconstructed AOD data, respectively. The <u>p</u>ercent numbers shown in the two left panels indicate <u>a</u> spatial coverage ratio of valid AOD retrievals over the selected scenes.

In Figure 3, we evaluated <u>the</u> impacts of <u>the</u> missing rate<u>of the target image AOD_{Terrr}</u> on the AOD gap-filling accuracy. By masking <u>raw-one truly observed AOD_{Terra} retrievals-image</u> with arbitrarily selected cloud masks, <u>thea series of AOD_{Terra} target</u> images under different missing rates, as shown in the top panel of Figure 3, were generated simulated and used as target images forfor gap-filling <u>trails(i.e., imagesas shown</u> in the top panel<u>of Figure 3</u>). The results showAs shown, <u>-anthe</u> reconstructed fields fairly agreed with<u>a</u> stronggood agreements between <u>the</u> observed and reconstructed. AOD fields, <u>well</u> resembling the actual AOD distribution over the outlined region, even <u>inover</u> extreme situations with excessive data gaps, demonstrating an excellent performance of the proposed gap-filling method. As expected, the reconstruction accuracy of the reconstruction fields decreased along with an increase in <u>the</u> missing rate. For instance, <u>when the missing rate was greater than</u> 80%, the low values in the upper left <u>in_of the</u> raw AOD_{Terra} image were not properly reconstructed when <u>the missing rate was greater than</u> 80%, largely because of the limited prior knowledge in the target image for use when constructing the raw AOD tensor. This effect also highlighting highlights the <u>vital-crucial</u> importance of prior information on the gap-filling accuracy. Therefore, increasing prior information is the most promising way to improve the <u>gap-filling</u> accuracy in <u>gap filling</u>, in particular for those areasregions with substantial data gaps.

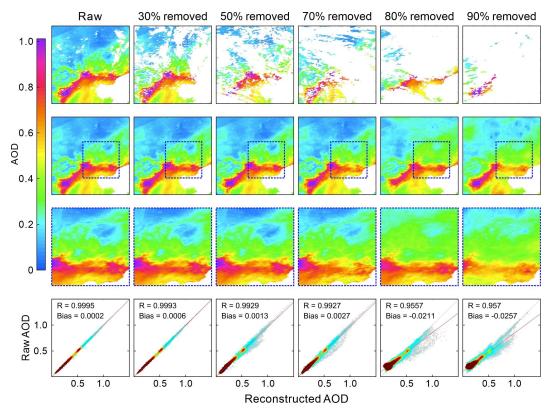


Figure 3. Impacts of <u>the</u> missing rate on the AOD gap-filling accuracy. <u>The nNumbers</u> on the top indicate the percentage of removed AOD data in <u>the</u> raw AOD_{Terra} image (top panel). The second row shows the distribution of <u>the</u> gap-filled AOD with zoom<u>ed</u>—in maps present in the third row. The bottom panel_presents scatter plots between <u>the</u> observed <u>AOD (withheld_raw_data)</u> and <u>the reconstructed AOD reconstructed from different inputs</u>.

4.2. Data AAAccuracy of Gglobal Ggap-Ffree AOD in LGHAP v2

The gap-free AOD grids dataset-(in the LGHAP v2) wasere generated by filling in data gaps in AOD_{Terra} images the satellite-based MAIAC AOD retrievals (MCD19A2) with reconstructed AOD estimates at each collocated footprint over land. In comparisonBy comparing against to the independent AOD observations from AERONET, the data accuracy of the gap-free AOD in the LGHAP v2 was comprehensively evaluated across the globe. Figures: 4a-c present athe spatial distribution of the site-specific correlation coefficient (R), root mean square error (RMSE), and bias between the reconstructed reconstructed AOD in the LGHAP v2 and AOD-AERONET observations from AERONET, respectively. Regardless of the uneven distribution of ground-based aerosol monitoring observing stations and the difference variations in data samples between sites, the ground validation results indicate a good agreements between the AOD in the LGHAP v2 and the AERONET observations, with an average of site-specific correlation coefficient of 0.76±0.14 and RMSE of 0.09±0.08 at theon a global scale. Meanwhile, the results indicate thatNote site-specific data accuracy metrics exhibit notable spatial heterogeneities-vary across the globeregions, with larger biases mainly observed in the central and east Asia as well as in Africa—regions frequently laways, which where often sufferings from high aerosol loadings.

Figures- 4d-4i present scatter plots between <u>the LGHAP v2gap-free</u> AOD and AERONET observations at six major continental regions. The distinct accuracy metrics across regions also indicate significant spatial heterogeneities in <u>the AOD</u> data accuracy. When compared against<u>to the AOD</u> observations from AERONET, <u>tAs shown</u>, <u>tThe</u> reconstructed AOD estimates were prone to <u>an underestimation of underestimate</u> large AOD observations <u>values</u> (>_0.80) <u>versus an</u>-whereas overestimat<u>ione of</u> low values (<_0.2) across these six regions. <u>ThisSuch an</u> effect is particularly common in <u>machine-machine-learning</u>, largely <u>because ofdue to</u> the imbalanced distribution of data values in <u>the</u> training samples (Johnson <u>and&</u>

Khoshgoftaar, 2019; Shi et al., 2022). Likewise<u>Similarly</u>, the inherent reason could be also applied fors for the this effect in tensor completion might be identical, which could be largely attributable to as the principle of low-rank approximation to fulfilfulfillrequired for tensor reconstruction and the imbalanced (i.e., few extremes) AOD values (i.e., few extremes) in the input tensor. Consequently<u>As a result</u>, the missed AOD extremes <u>could may not be accurately</u> were hardly to be reconstructed to their nominal levels; <u>iInsteadRather</u>, they tend the reconstructed values were inclined to resemble a mean state that was determined by principal modes via a low-rank approximation. <u>because ofdue to the imbalanced data distribution</u>.

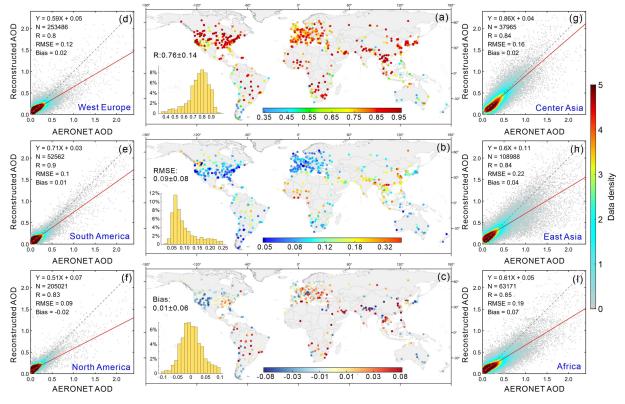


Figure 4. Data accuracy of daily gap-free AOD grids in <u>the</u> LGHAP v2 dataset <u>compared</u>by <u>comparing againstto</u> <u>the</u> AOD observations from AERONET across the globe during 2000–2021. Note <u>the</u> AERONET AOD observations were independent data <u>from and had been not</u> <u>used in</u> the gap-filling process.

To <u>further</u> verify the data accuracy of <u>the</u> imputed AOD estimates, we-<u>further</u> compared the <u>data accuracy of gap-filled</u> AODs in <u>the</u> LGHAP v2 dataset with two major gridded products, i.e., <u>of satellite-based_MAIAC AOD retrievals from Terra</u> (<u>AOD_{Terra}MCD19A2</u>) and <u>downsealed MERRA-2 AOD</u> (AOD_{M2}). As shown in Table 2, the purely reconstructed AOD estimates have <u>an</u> R of 0.83 and <u>an</u> RMSE of 0.15 compared <u>toggainst the</u> AERONET AOD observations at the global scale______, comparable to the data accuracy of AOD_{M2} (R_=_0.83, RMSE_=_0.14) but lower than that of AOD_{Terra} (R_=_0.88, RMSE_= 0.11). Nevertheless, the imputed AOD estimates achieved comparable data accuracies <u>togs</u> AOD_{Terra} in Africa (R_=_0.80, RMSE_=_0.20) and Australia (R_=_0.62, RMSE_=_0.08), largely <u>because of the availability ofdue-to</u> abundant satellite-based AOD prior informationretrievals over these two areas (refer to the AOD coverage ratio shown in Figure S1) to facilitate AOD gap-filling via-tensor completion. In contrast, the <u>LGHAP v2imputed</u> AOD estimates in Europe and Asia have poorer data accuracies with relative to AOD_{Terra}, <u>particularlyespecially</u> in <u>Eastern</u> Asia. The <u>p</u>Possible reasons<u>-for this</u> could be ascribed to not only extensive missing values, severe aerosol pollution levels, as well as significant spatial variations in aerosol loadings over these regions. Compared to AOD_{Terra}MAIAC AOD, the gap-filled AOD data tended to overestimate the AERONET AODs (17.59% versus 11.45% above the envelope of expected error), resulting in the usen larger global mean AOD values were reconstructed in the imputed AOD estimates.

<u>Moreover, the accuracy of The gap free AOD dataset (LGHAP v2) was generated by filling in data gaps in the satellite-based AOD retrievals (MCD19A2) with reconstructed AOD estimates at each collocated footprint over land. The gGround validation results indicate that the gap-filled AOD data in LGHAP v2 are in a good agreement with the AERONET AOD observations, with an R of 0.85 and an RMSE of 0.14 across the globe (Table 2)__, slightly worse than that of raw MCD19A2 (R_=0.88 and RMSE_=0.11) but higher than that of AOD_{M2} (R_=0.83 and RMSE_=0.14). This dataLGHAP v2 AOD data accuracy-outperforms that of the gap-filled AOD dataset (R²=0.6031 and RMSE_=0.1350) generated by Guo et al. (2023), in which missing AODs in MCD19A2-AOD_{Term}MAIAC were predicted with using versatile various proxy variables (e.g., meteorological factors and population density) via a random forest model.</u>

Table 2. An intercomparison of AOD data accuracy between satellite-based retrievals (raw MAIAC AOD), numerical aerosol diagnostics (downscaled MERRA-2 AOD), purely reconstructed data, and the final gap-free product (LGHAP v2 AOD), by comparing AOD observations from AERONET across the globe during 2000–2021. Note the term "Purely Reconstructed AOD" refers to the imputed AOD estimates, while "LGHAP v2" refers to the gap-filled AOD dataset combining both satellite-based retrievals and purely reconstructed data. The expected error (EE) envelope for AOD over land was defined as $\pm (1.5 \times AOD_{AERONET} \pm 0.05)$.

AOD Dataset	Region	Mean AOD	Number of Monitors	Number of Samples	R	RMSE	Bias	Below EE (%)	Within EE (%)	Above EE (%)
	Global	0.17	1,335	402,886	0.88	0.11	0.02	13.95	74.59	11.45
	North America	0.11	433	112,438	0.83	0.08	-0.01	4.62	80.93	14.44
	South America	0.11	81	28,265	0.94	0.07	0.02	14.17	75.85	9.97
MAIAC (AOD _{Terra})	Europe	0.11	208	96,715	0.80	0.06	0.02	11.29	82.22	6.49
	Asia	0.31	321	90,821	0.90	0.14	0.02	18.79	68.22	12.99
	Africa	0.21	110	48,877	0.81	0.19	0.06	31.45	57.11	11.44
	Australia	0.09	28	12,427	0.62	0.07	-0.01	6.16	75.34	18.49
	Global	0.18	1,335	811,438	0.83	0.14	0.02	11.76	78.98	9.26
	North America	0.12	433	216,264	0.80	0.09	0.00	5.71	86.22	8.07
Downscaled	South America	0.13	81	49,721	0.90	0.11	0.02	12.87	81.64	5.49
MERRA-2	Europe	0.13	208	177,125	0.79	0.07	0.01	8.54	86.07	5.39
(AOD _{M2})	Asia	0.29	321	175,781	0.78	0.24	0.06	22.54	65.14	12.32
	Africa	0.24	110	88,374	0.85	0.15	0.02	16.13	67.59	16.28
	Australia	0.10	28	21,051	0.76	0.06	-0.02	2.44	83.60	13.96
	Global	0.21	1,335	449,452	0.83	0.15	0.01	12.21	65.52	22.27
	North America	0.16	433	129,716	0.80	0.10	-0.02	5.23	67.52	27.25
Purely	South America	0.17	81	30,073	0.88	0.11	0.00	10.51	67.11	22.38
Reconstructed	Europe	0.16	208	107,961	0.73	0.09	0.00	9.63	73.63	16.74
AOD	Asia	0.33	321	107,876	0.81	0.24	0.03	18.64	56.60	24.76
	Africa	0.27	110	31,568	0.80	0.20	0.06	29.57	53.88	16.55
	Australia	0.13	28	9,628	0.62	0.08	-0.03	4.60	64.62	30.77
LOUIAD-2	Global	0.19	1,335	756,166	0.85	0.14	0.01	12.96	69.44	17.59
	North America	0.13	433	216,055	0.82	0.09	-0.01	4.86	73.12	22.02
	South America	0.14	81	49,707	0.90	0.10	0.01	12.57	71.08	16.34
LGHAP v2	Europe	0.13	208	176,959	0.76	0.08	0.01	10.24	77.40	12.36
	Asia	0.32	321	175,728	0.83	0.21	0.03	19.08	61.40	19.52
	Africa	0.23	110	75,110	0.81	0.19	0.06	29.61	56.64	13.75

In Figure 5, we compared temporal variations in AOD between the LGHAP v2 dataset and AERONET-ground-based observations at six <u>AERONET aerosol-observing</u>-sites with long-term monitoring-records. Compared to discrete AOD observations from AERONET, the gap-free AOD time series accurately well-reconstructed long-term variations of aerosol loading from 2000 to 2021 at these-six monitoring sites, with R ranging from 0.83 to -0.97 and RMSEs varying between 0.04 and 0.24. Note that tFhe lLarger RMSEs observed at the Alta Floresta and Beijing sites are more likely ascribed to the reconstruction failures of extreme-abnormal AOD peaks, largely because of very limited peak values for reference in the AOD tensor. Referring to histograms of AOD deviations between the LGHAP v2 and AERONET observations, more than 80% of AOD biases fell within the range of were found to vary between -0.1 and to 0.1, demonstrating a high accuracy of the gap-free-filled AOD in the LGHAP v2 dataset.

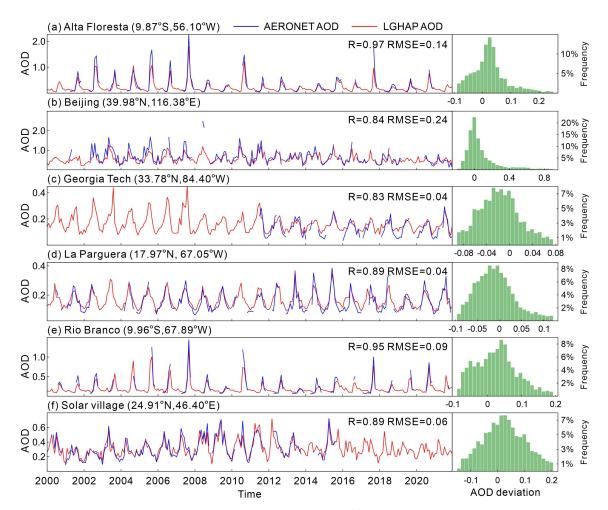


Figure 5. Temporal variations in <u>the</u> monthly AOD over six AERONET sites with long-term AOD observations <u>during from 2000-to 2021</u>. <u>The p</u>Panels on the right present histograms of AOD deviations between <u>the</u> LGHAP v2 and AERONET observations at each individual site.

4.3. Data Aaccuracy of Gglobal Ggap-Ffree PM2.5 Ceoncentrations in LGHAP v2

Global gap-free PM_{2.5} concentration estimates were then derived from gap-filled AOD images by taking advantage of the novel <u>SCAGAT</u> modelethod that was specifically developed to <u>fulfilfulfill</u> thefor global PM_{2.5} concentration mapping. <u>AdditionalMore</u> details related to the performance evaluation of the SCAGAT model_method were described_provided in another companion_study (Li et al., 2024), and here we-hereby focused on the data accuracy of the global gap-free PM_{2.5}

concentration estimates. Figure 6 presents the validation accuracy of the daily gap-free PM_{2.5} concentration estimates by comparing them against to the ground-based PM_{2.5} concentration records measured at 350 independent (previouslypriorly) hoeld-out) monitoring sites. The results As indicated, by accounting for spatial representativeness of the prediction models during the spatial extrapolation, that PM2.5 concentration estimates derived from the SCAGAT model are inhave better better agreements with ground measured -based PM2.5 concentration measurements across the globe (, with an R = of 0.91 and an RMSE =-of 9.587 µg m⁻³), outperforming surpassing the performance of our traditional PM2.smachine-learning ed prediction models without accounting for the spatial representativeness of the prediction models during the spatial extrapolation (Bai et al., 2019, 2022a, 2023). Meanwhile, As shown in Figure 6e, by taking advantage of the SCAGAT model, the PM_{2.5} concentration estimates over China in LGHAP v2 have a higher data accuracy (R = 0.97, RMSE = 7.93 µg m⁻³) than those in LGHAP v1 (R_-0.95, RMSE_-12.03 µg m⁻³), neglecting <u>a different number of validation samples.</u> (The data accuracy was further improved by correcting modelling biases using sparsely distributed in_-situ PM2.5 concentration measurements via optimal interpolation, where resulting in an improvement in with R improved to 0.95 and a reduction decrease in RMSE-was reduced down to 5.7 µg m⁻³ (as shown in Figure 6b). As shown in Figure 6e, by leveraging the SCAGAT model, the PM_{2.5} concentration estimates over China in the LGHAP v2 have a higher data accuracy (R = 0.97, $RMSE = 7.93 \mu g m^{-3}$) than those in LGHAP v1 (R = 0.95, RMSE = 12.03 μ g m⁻³), Figuress. 6c-6d present a site-based distribution of R and RMSE for the LGHAP v2 PM_{2.5} concentrations over each individual validation site. Compared to the United States of America and Europe, as shown depicted in Figures- 6e-6g, larger PM2.5 concentration biases were more likely to be observed in Asia China because of due to thegiven higher PM2.5 loadings therein.

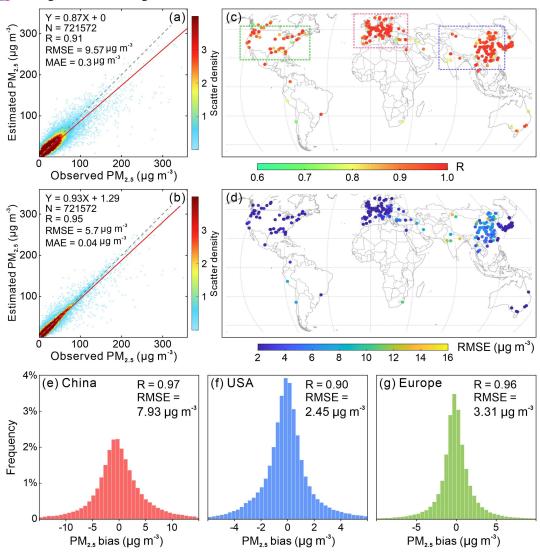


Figure 6. Site-based validation accuracy of PM_{2.5} concentration estimates derived from gap-free AOD images using the proposed SeGAT <u>SCAGAT</u> method₂, (a) Scatter plots between PM_{2.5} estimates derived from the <u>SeGAT-SCAGAT</u> model and <u>the withheld ground-based</u> PM_{2.5} concentration measurements. (b) Same as <u>Figure. 6(a)</u> but for gap-free PM_{2.5} estimates fusing ground measured PM_{2.5} concentration measurements. (c–d) Site-based correlation coefficient and RMSE for LGHAP v2 PM_{2.5} concentrations, respectively. (e–g) Histograms of LGHAP v2 PM_{2.5} concentration bias over China, United States, and Europe, respectively. Note <u>the</u> ground-based PM_{2.5} concentration data used here for validation <u>were held out priorly and used neitherwere as not involved in-used neither in the</u> model training nor <u>in the</u> data fusion procedures.

Table 3 presents <u>the</u> data accuracy of <u>the</u> gap-free PM_{2.5} concentrations in <u>the</u> LGHAP v2 dataset during the period of 2000–2021 over nations with adequate sufficient records of ground-based measurements of PM_{2.5} concentration measurements records. It indicates that the data accuracy of PM_{2.5} concentration estimates varied across regions, with R changing from 0.71 to 0.98 and RMSEs ranging between 1.15 and 32.69 µg m⁻³. Regardless of <u>the</u> substantial differences in <u>the</u> total number of data pairs across regions, larger RMSEs are mainly observed in regions like Mongolia (32.69 µg m⁻³) and India (25.34 µg m⁻³), which where often suffered from high-severe PM_{2.5} loadingspollution episodes. The spatially varying accuracy metrics between regions not only highlight the great complexity in large-scale PM_{2.5} modeling. This, which also andbut-underscores the critical importance of <u>consideringaccounting for</u> spatial representativeness via data driven models, when applying models over other regions for data extrapolation.

In Figure 7, we examined long-term variations in PM_{2.5} concentrations in four different cities during from 2000-to 2021. The A good agreement between the LGHAP v2 PM_{2.5} concentration time series andwith the unseen (previously withheld) ground based PM_{2.5} concentration measurements confirms the significant/demonstrated a high accuracy of the LGHAP v2 PM_{2.5} concentration datasetestimates. Compared to temporally discrete PM_{2.5} concentration records measured by ground monitors, the gap-free LGHAP v2 PM_{2.5} concentration time series enabled us to examine better understand the long-term variability of haze pollutions across the globe, benefiting from its given the gap-free merit. Additionally, the agreement between the LGHAP v2 PM_{2.5} concentration time series and the unseen (previously withheld) ground-based PM_{2.5} concentration dataset confirm the significant accuracy of the LGHAP v2 PM_{2.5} concentration dataset. Therefore, this gap-free PM_{2.5} concentration dataset can be used with confidence when assessing long-term trends of haze pollution across the globe. As shown, declining trends in PM_{2.5} concentration were observed in PM_{2.5} concentrations as early as in 2006 in New York (United States), whereas apparent reductions were mainly observed mainly after 2012 in Jilin (China) and 2015 in Toyama (Japan). Overall, the gap-free and high accuracy merits render PM_{2.5} concentrations in the LGHAP v2 dataset reliable data sources for assessing long-term trends of haze pollutions across the globe.

Table 3. The dData accuracy of gap-free $PM_{2.5}$ concentrations in the LGHAP v2 dataset by compareding togainst ground-based $PM_{2.5}$ concentration datameasurements in countries with adequate sufficient $PM_{2.5}$ concentration measurements records. The N denotes the total number of $PM_{2.5}$ concentration data pairs for calculating R, RMSE₄ and bias.

Country	Ν	R	RMSE (µg m ⁻³)	Bias (µg m ⁻³)	Country	Ν	R	RMSE (µg m ⁻³)	Bias (µg m ⁻³)
China	3,113,160	0.97	8.27	0.36	Iran	67 <u>,</u> 434	0.74	10.14	-0.09
USA[NC1]U nited States	2_048_983	0.84	3.34	0.06	Brazil	50,252	0.81	5.63	0.78
Japan	1_810_436	0.96	1.82	0.07	Portugal	47,782	0.82	3.49	0.14
Canada	1_206_176	0.89	2.12	0.05	Hungary	41_524	0.92	4.59	-0.17
Korea	526_138	0.96	3.49	0.16	Sweden	40 <u>.</u> 839	0.91	1.61	-0.23
France	502,555	0.96	2.25	0.13	Norway	40,001	0.86	2.45	-0.07

Germany	472_103	0.97	1.94	0.04	Finland	38 <u>.</u> 884	0.93	1.15	-0.08
Italy	371_888	0.93	5.23	0.04	South Africa	35,314	0.71	10.84	-2.91
UK United <u>Kingdom</u>	309,181	0.94	1.95	0.11	Serbia	34,795	0.87	9.70	0.01
Spain	297,202	0.87	2.63	0.23	New Zealand	26,654	0.73	3.63	0.20
Czech <u>Republic</u>	209,274	0.97	3.38	0.24	Colombia	26,332	0.95	4.60	0.45
Australia	208,772	0.72	3.70	-0.03	Ukraine	22,692	0.84	5.79	-0.08
India	207,974	0.92	25.34	1.64	Bosnia- Herzegovina	20,297	0.94	12.08	1.59
Belgium	177 <u>.</u> 036	0.98	1.54	0.01	Greece	19 <u>.</u> 410	0.79	5.41	-0.10
Poland	175,782	0.95	5.03	0.52	Croatia	17,926	0.90	5.82	-0.44
Turkey	171 <u>,</u> 381	0.84	10.27	-0.99	Switzerland	14,719	0.75	3.98	-2.26
Austria	131,186	0.97	2.28	-0.14	Russia	14_357	0.84	4.06	0.58
Netherlands	119,047	0.97	1.72	-0.07	Estonia	13_793	0.91	1.48	0.19
Mexico	112_379	0.80	11.42	0.45	Lithuania	13_405	0.87	4.49	0.07
Chile	111 <u>,</u> 416	0.80	12.64	0.16	Ecuador	12,517	0.88	2.92	0.28
Slovakia	104_892	0.95	3.77	0.18	Vietnam	12_480	0.78	12.94	0.63
Thailand	82_206	0.89	13.21	1.25	Macedonia	10 <u>,</u> 416	0.92	10.81	2.17
Israel	68,012	0.83	5.08	0.32	Mongolia	9,926	0.91	32.69	-0.17

Figure 8 presents the temporal variations in the global annual mean PM_{2.5} concentration distribution from 2000 to 2021. First of allFirstAs shown, the daily gap-free merit of the LGHAP v2_dataset-can seamlessly supports the derivation of comparable annual mean PM_{2.5} concentration maps between years, as and data gap related biases in raw AOD_{Terra} images were eliminated because of due to the usage of daily gap-free PM_{2.5} concentration data. HoweverOn the other hand, tMeanwhile, the quality-assured annual mean PM_{2.5} concentration maps enable us not only to easily pinpoint the hotspot regions suffering from severe haze pollutions andbut also to examine analyze the long-term variability of global PM_{2.5} concentrations across the globe. Specifically, As shown, Mongolia, north India, eastern China, and central Africa were identified as four major regions with relatively high PM_{2.5} loadings, in particular north India, becoming a hotspot region suffering from more severe PM_{2.5} pollutions on the planet. Substantial PM_{2.5} reductions were observed in eastern China since-from 2014_onwards, with PM_{2.5} concentrations reduced to a levels even comparable to countries in central Asia;, and in turnhowever, north India was_in turn athe hotspot region experiencingsuffering from more severe PM_{2.5} pollutions on the planet.

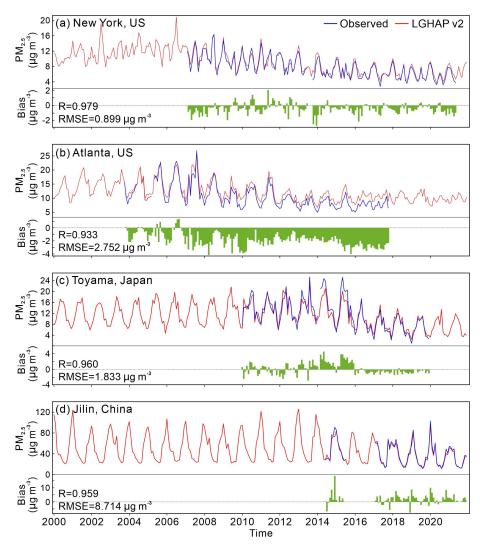


Figure 7. An inter-comparison of temporal variations in monthly <u>mean PM_{2.5} concentrations</u> in four different cities between <u>the LGHAP v2</u> and collocated ground-based $PM_{2.5}$ <u>concentration</u> measurements <u>during from 2000= to 2021</u>.

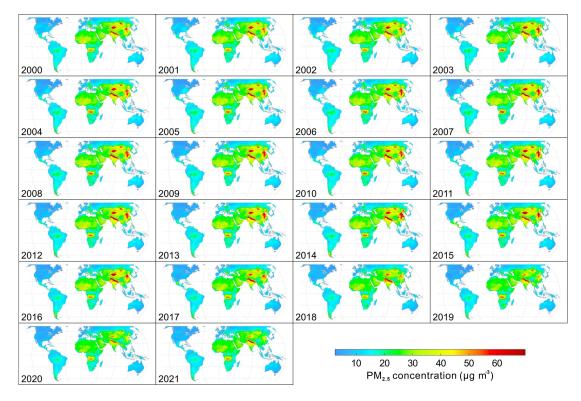


Figure 8. Spatial distribution of the global annual mean PM_{2.5} concentrations derived <u>using from</u> the LGHAP v2 dataset <u>from between 2000</u> to and 2021.

5. Discussion

Spatially contiguous AOD and PM_{2.5} concentration grids are pivotal to regional air quality management, haze pollution exposure risk assessment, and aerosol radiative forcing diagnosis. By seamlessly gearing up state-of-the-art machine_-learning and tensor completion methods, a novel framework of big earthEarth data analytics framework was developed to fulfill the generation of long-term high-resolution AOD and PM_{2.5} concentration grids as of 2000 in China-(LGHAP v1) in our previous study (Bai et al., 2022a).-MultimodalSpecifically, multimodal AODs and relatedevant air quality measurements-data acquired from diverse satellites, numerical models, and ground monitoring stations were firstly harmonized using random forest-based data-driven models. Next, mMultisource AOD data flows were then-weaved neatly as the tensor inputs_a; from andwith which data gaps in daily MODIS AOD imageries were properly reconstructed via low-rank tensor completion. Finally, gap-free PM_{2.5} concentration grids were mapped from gap-filled AODs-AOD images using a random forest model-through machine-learned regression models. This big data analytics framework provided an effective solution to integrate multimodal earthEarth observations from diverse two gap free datasets also well demonstrated the efficacy of this framework.

In this study, aiming to generate global gap-free AOD and PM_{2.5} concentration grids, namely the LGHAP v2 dataset, the previous big earthEarth data analytics framework proposed in our previous study was adopted but enhanced with several new featuresto generate global gap-free AOD and PM2.5 concentration grids, i.e., the LGHAP v2 dataset. Similarly, HOSVD was applied as the core method for tensor completion to fulfill the AOD gap filling. Despite similar data manipulation procedures, sSeveral new algorithmic enhancement modules were also implemented, with particular focuses on to accommodatinge the rocketing data size and global scale modeling demand, aiming, not only to improve the computing efficiency and other than but also to reduce reducing modeling biases. Specifically, an attention mechanism, inspired by deep-learning techniques, was hereby introduced to weight each data slice in the input tensor to account for the drawback induced by Likewise, HOSVD was applied as the core method for tensor completion to fulfilfulfill the AOD gap filling. Nonetheless, previous results indicated a potential drawback as an the equal weight of each data slice in the AOD data cube rendered strategy, with, with llLarger weights were assigned to data slices that better resembleding with fewer data gaps and more similar to the actual AOD distribution target image on the target date with more valid observations. In such a research contextother words, both the spatial coverage ratio of valid observations in each soft data and the mutual information between the target and soft data were usedserved as two relevant metrics were considered simultaneously to help determine the weight assigned to each data slice in the AOD tensor. A weighted AOD tensor was then calculated and used as the input tensor data to compel guide for tensor completion process, prioritizing focuseding on data slices more similar tolikeclosely resembled the target image rather thainstead of n using all the available datainformation in the AOD tensor indifferently. As demonstrated by Although the ablation experiments shown in Figure 2,- have demonstrated the efficacy of the AOD fields reconstructed from the this attention-reinforced tensor better resembled the actual AOD distributions in the target MODISt AOD Terra images than those derived from the raw original AOD tensor without applying the attention mechanism construction strategy, the underlying philosophy, in particular the relative importance of mutual information and extra spatial coverage, has been not yet fully justified and assessed.

Meanwhile, a<u>A</u>n adaptive background field updating scheme was <u>also</u> introduced to <u>iteratively</u> update prior information in the target AOD_{Terra} images <u>during each iteration of tensor decomposition and reconstruction</u>, and the<u>The</u> ultimate <u>goalobjectivegoal</u> was to mitigate the influence of prior information on the reconstruction accuracy, particularly reducing the probability <u>risk of possible propagation of large modelling biases from background</u> in AOD_{M2} to the reconstructed AOD fields. Compared to the invariant prior information, adaptively updated prior information <u>allowed for mitigating the influence of</u> <u>uncertainties in the prior information on the reconstruction accuracy</u>, particularly large modeling biases from numerical enabled us to not only improve the<u>d</u> reconstruction efficiency <u>and</u> but also significantly reduced the probability of large error propagation from numerical AOD simulations. Despite these algorithmic improvements, the inter-comparison results even indicated a slightly reduced data accuracy of gap-filled AODs in China from the LGAHP v2 dataset was observed compared to those in the LGHAP v1 dataset. Further investigations revealed this was mainly due to the<u>a</u> relatively poor data accuracy of the downscaled AOD_{M2} data <u>because since abecause a</u> global-scale <u>versus</u> rather than regional downscaling model was applied to harmonize AOD_{M2} in China. This<u>i</u> in turn<u>i</u> underscores the vital importance of data cleaning procedures on reducing the bias levels of each supplementary data to manage the total error budget in the final analyzed data fields when performing big data analyties. Nonetheless, benefiting from the adaptive background updatinge scheme, the modeling biases in AOD_{M2} background AOD fields were effectively mitigated suppressed in the final reconstructed AOD fields, evidenced by larger biases of AOD_{M2} (R = 0.77, RMSE = 0.36) versus smaller biases of the purely reconstructed AOD (R = 0.82, RMSE = 0.26).

As illustrated in Figure 9, the The global gap-free and high-resolution benefits _gap filled AOD grids with a daily 1 km resolution enable us render the LGHAP v2 dataset a promising data source to better monitor global aerosol distribution and variations in space and time. Aerosol-As illustrated in Figure 9, aerosol-related environmental disturbance episodes, such as sandstorms, wildfires, and haze pollution events, can be well indicated by local rising AODs at the regional seale. More importantlyst critically, the gap-filled AOD dataset provides us with an unprecedented opportunity to monitor aerosol loadings and variations even under cloud covers, e.g., the haze pollution episodes over southern India and eastern China shown in Figures 9d and 9e₂₅ This is largely benefited _from the the intelligent spatiotemporal pattern recognition and learning, as well as the assimilation of air quality measurements from ground monitoring stations and numerical aerosol diagnostics. While thissuch a global air quality mapping approach greatly facilitates the surveillance and management of air pollution around the world, the high resolution gap free AOD and PM_{2.5} concentrationLGHAP v2 dataset would also largely significantly reduce the uncertainty-uncertainties in the health-related aerosol exposure risk assessment results because of the gap-free and high-resolution advantages.

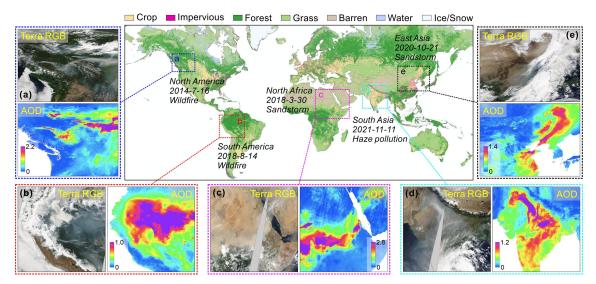


Figure 9. An illustration of AOD responses to wild firewildfires, sand storms and storms, and haze pollution episodes across the globe, as characterized by gap-free AOD in the LGHAP v2 dataset. The gGlobal map in the middle panel shows athe spatial distribution of the major land cover types in 2020.

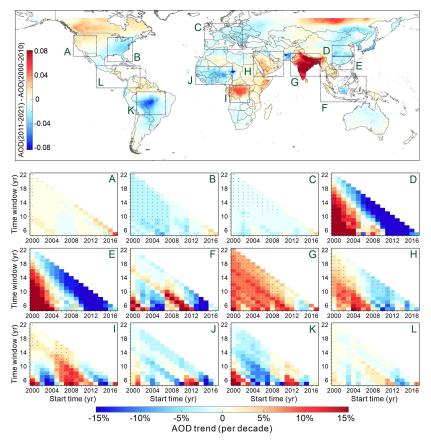


Figure 10. AOD trends over twelve regions of interest <u>across the globe worldwide</u> from 2000 to 2021 estimated from gap-free AOD_S in the LGHAP v2 dataset. The top panel shows <u>a-the</u> spatial distribution of global AOD deviations between the first and second decade in the 2000s. Twelve diagrams in the bottom panel show the linear trend of mean AOD over the outlined region of interest at different starting times with varying time window sizes.

<u>Global AOD variation trends were carefully examined by</u>By taking advantage of the LGHAP v2 AOD dataset, <u>global</u> AOD variation trends were carefully examined. Figure: 10a presents <u>the</u> AOD deviations between <u>the</u> AOD averages during the first and the second decade <u>in 2000s</u> across the globe. As shown, substantial AOD increases in the <u>twenty-first21st</u> century present-primarily <u>present</u> over India (G)_and central Africa (I), with remarkable AOD decreases observed in the middle of South America. In North America, AOD increases were mainly observed in Canada and <u>the</u> western <u>United StatesUS (A)</u> whereas AOD decreases were found in <u>the</u> eastern <u>United StatesUS (B)</u>. <u>Additionally</u>, <u>Also</u>, <u>in referencereferring</u> to temporally varied varying AOD trends in regions A and B, we may observe evident AOD increasing trends <u>have beenwere observed</u> in the <u>United StatesUS fromsince</u> 2012 <u>onwards</u>, while <u>the</u> significant decreasing trends in <u>the</u> eastern <u>United StatesUS</u> were even totally<u>entirely</u> reversed after 2015. This effect could be partially <u>linked_attributed</u> to more frequent and intensive wildfire emissions <u>in north America</u> in <u>during</u> the second decade of <u>the</u> 2000s in north America (Burke et al., 2023; Wei et al., 2021b). <u>A s</u>Similar effect was also observed in Europe (C), with an apparent slowdown in <u>the</u> AOD decreasing trend after 2010.

<u>IApparent</u> inverse effects were also observed in China but with totally different temporal transition patterns. As shown, statistically significant AOD increasing trends were observed in eastern (D) and southern (E) China in the first decade, whereas increasing trends started to slow down since 2007 with a slowdown starting around 2007, and followed by a sudden reversione to decreasing trends was observed after 2010. More importantly, <u>T</u> this was also the most significant AOD decreasing trend in <u>during the</u> 2010s around the world. Thisese observational evidences <u>confirmsaffirm</u> the great-success of clean air actions in improving air quality in China during the pastrecent decades (Bai et al., 2022a; Liang et al., 2020; Zhang et al., 2019). <u>A</u> <u>S</u> Similar temporal variation pattern was also observed in <u>the</u> Middle East (H) but with relatively weak trends. In contrast, India

(G) was <u>athe</u> hotspot area showing an increasing trend in AOD throughout the 2000s, despite a short period of increasing hiatus <u>fromduring</u> 2013–<u>to</u> 2015.

In this study, <u>gG</u>lobal gap-free PM_{2.5} concentrations were derived <u>on the basis ofbased on</u> gap-filled AOD grids by taking advantage of a novel SCAGAT <u>deep_learning</u>-model, which was specifically developed to fulfil<u>fulfill</u> global <u>global_scale</u> PM_{2.5} concentration mapping. Differing from<u>Unlike</u> many other <u>data-driven</u> modeling practicess, the spatial representativeness of data driven models was accounted for by in the SCAGAT <u>model</u>, providing a unique solution to model PM_{2.5} concentration<u>s</u> over regions even without PM_{2.5} monitoring sites. The availability of <u>dD</u>aily gap-free PM_{2.5} concentration grids <u>also</u> favor<u>§</u> the assessment of <u>the</u> pandemic's <u>influence</u>-impacts on regional air quality. Fig<u>uress</u>. 11a and 11b₂ in the middle panel₂ present <u>athe</u> spatial distribution of PM_{2.5} concentration<u>s</u> before and during the COVID-19 pandemic, respectively. Neglecting longterm variation trends in PM_{2.5} concentration<u>s</u>, the substantial PM_{2.5} decreases in <u>the</u>-middle and eastern China₁ as well as <u>in</u> central Europe₁ clearly indicate the positive effect of <u>pandemic</u>-pandemic-related mobility restrictions on air quality improvement₇ (by comparing PM_{2.5} concentration in 2019 and 2020 during the synchronous period). In contrast, PM_{2.5} reductions were relatively small in <u>the United States</u>US due to the lack of mobility restriction measures, with apparent PM_{2.5} reductions observed mainly in <u>regions like</u> Chicago. Overall, <u>the availability of the</u> LGHAP v2 dataset enables us to better investigate global aerosol variations and <u>to assess assess</u> PM_{2.5-5-5}-related health <u>exposure</u> risk<u>s</u>-via <u>exposure assessment</u>.

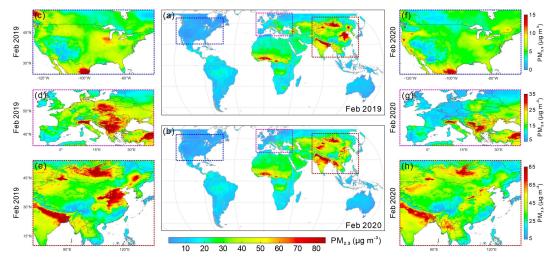


Figure 11. Influencempacts of the COVID-19 pandemic on $PM_{2.5}$ concentrations in United States, Europe, and China. The $PM_{2.5}$ concentrations from LGHAP v2 were averaged over athe synchronous periods in 2019 and 2020 for inter-comparison.

6. Data Availability

The LGHAP v2 dataset provides global gap-free AOD and PM_{2.5} concentration grids from 2000 to 2021 with <u>a</u> daily 1km resolution. To facilitate <u>the</u> data sharing, each daily map was saved <u>as one a separateingle</u> NetCDF file, and <u>the</u> data in each individual month wasere then archived as <u>a one</u> zip file. <u>Because ofDue to the data storage limitations, one year of data</u> in one year were archived as one single dataset. Table 4 provides <u>summarizes</u> the permanent digital object identifiers for <u>data</u> in each individual_datasetcalenda year from 2000 to 2021. All these datasets were <u>publicly</u> available at the LGHAP community link via <u>https://zenodo.org/communities/ecnu_lghap</u> (Bai et al., 2023a). <u>The d</u>Data user guide and visualization codes (Python, MATLAB, R, and IDL) were also provided to guide the users <u>inte</u> retrievinge data from the NetCDF files, which can be accessedible at <u>https://doi.org/10.5281/zenodo.10216396</u>.

Table 4. List of data links for AOD and PM2.5 concentration grids in the LGHAP v2 dataset for each individual year.

Year	LGHAP v2 AOD grids	LGHAP v2 PM _{2.5} grids
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2000	https://doi.org/10.5281/zenodo.8281206	https://doi.org/10.5281/zenodo.8307595
2001	https://doi.org/10.5281/zenodo.8281216	https://doi.org/10.5281/zenodo.8307597
2002	https://doi.org/10.5281/zenodo.8281218	https://doi.org/10.5281/zenodo.8307599
2003	https://doi.org/10.5281/zenodo.8281222	https://doi.org/10.5281/zenodo.8307601
2004	https://doi.org/10.5281/zenodo.8281226	https://doi.org/10.5281/zenodo.8307605
2005	https://doi.org/10.5281/zenodo.8281228	https://doi.org/10.5281/zenodo.8307607
2006	https://doi.org/10.5281/zenodo.8287125	https://doi.org/10.5281/zenodo.8308225
2007	https://doi.org/10.5281/zenodo.8287129	https://doi.org/10.5281/zenodo.8308227
2008	https://doi.org/10.5281/zenodo.8287133	https://doi.org/10.5281/zenodo.8308231
2009	https://doi.org/10.5281/zenodo.8287995	https://doi.org/10.5281/zenodo.8308233
2010	https://doi.org/10.5281/zenodo.8288389	https://doi.org/10.5281/zenodo.8308237
2011	https://doi.org/10.5281/zenodo.8288395	https://doi.org/10.5281/zenodo.8310586
2012	https://doi.org/10.5281/zenodo.8288397	https://doi.org/10.5281/zenodo.8310590
2013	https://doi.org/10.5281/zenodo.8287207	https://doi.org/10.5281/zenodo.8310702
2014	https://doi.org/10.5281/zenodo.8288387	https://doi.org/10.5281/zenodo.8310704
2015	https://doi.org/10.5281/zenodo.8289613	https://doi.org/10.5281/zenodo.8310706
2016	https://doi.org/10.5281/zenodo.8289615	https://doi.org/10.5281/zenodo.8310708
2017	https://doi.org/10.5281/zenodo.8294100	https://doi.org/10.5281/zenodo.8310711
2018	https://doi.org/10.5281/zenodo.8301364	https://doi.org/10.5281/zenodo.8313603
2019	https://doi.org/10.5281/zenodo.8301367	https://doi.org/10.5281/zenodo.8313611
2020	https://doi.org/10.5281/zenodo.8301375	https://doi.org/10.5281/zenodo.8313613
2021	https://doi.org/10.5281/zenodo.8301379	https://doi.org/10.5281/zenodo.8313615

7. Conclusion

In this study, the LGHAP v2 dataset, a heritage of the LGHAP₋, which provides long term gap free AOD and PM concentration grids with <u>a</u>_daily 1 km resolution in China, was generated to provide <u>global_gap-free</u> AOD and PM_{2.5} concentration grids <u>with a daily 1-km resolution</u> with the same resolutionfrom 2000 to 2021-(as of 2000daily and 1km) across the globe), by taking advantage of <u>leveraging</u> an improved big <u>earthEarth</u> data analytics approach. The <u>gG</u>round validation results <u>demonstrate confirm</u> high accuracies of these two gap-free products, with AOD having a correlation<u>nan R</u> of 0.85 and an RMSE of 0.14 compared to the AERONET AOD observations₃₅ which are slightly worse than the original MCD19A2 product (R=0.88 and RMSE_=0.11). Similarly, The <u>sSite based validation</u> results also indicate that <u>the</u>PM_{2.5} concentration estimates derived from gap-free AOD via the SCAGAT method show <u>ana good</u> agreement with the withheldheld-out ground-based PM_{2.5} measurements, with_achieving an R of 0.91 and an RMSE of 9.57 µg m⁻³, and <u>Furthermore</u>, while the data accuracy was further-improved to <u>an R of</u> 0.95 and <u>an RMSE of</u> 5.7 µg m⁻³ with the fusion of ground-measured PM_{2.5} measurements. To our knowledge, this is the first two-decade-longtwenty-year global gap-free AOD and PM_{2.5} concentration.

<u>The dData gaps in satellite-based AOD images were filled using a similar Several new algorithmic enhancement modules</u> were incorporated to the big data analytics approach framework to what wasthat as developedused improve both the computing speed and the reconstruction accuracy to for generatinge the LGHAP dataset in China, albeitbut with several new algorithmic improvements. The ablation experiments well-demonstrated the effectiveness and advantages of applying incorporating-the newly implemented attention mechanism to weight each slice of soft data in the AOD tensor-during the tensor completion procedure. Also,Additionally, uUpdating prior information in the target image after each tensor reconstruction iteration not only helpsed mitigate the probability-risk of error propagation from numerical aerosol diagnostics to the final reconstructed field-<u>andbut also , while also and</u> improveinges the convergence speed of tensor completion. <u>MoreoverOverall</u>, this study provides a <u>good-compelling</u> illustration of big <u>earthEarth</u> data analytics to generate high-quality remote sensing datasets by synergistically integrating and assimilating multimodal data from diverse sources via <u>machine-machine-learning techniques</u>. The last but not leFastinallyAdditionally, this big data analytics approach can could be also used for be also used to fulfilfulfill near-term gap-free AOD mapping by <u>leveraging</u>simply replacing by simply replacing acrosol reanalysis with numerical AOD reanalysis with forecasting fieldss (e.g., CAMS AOD forecasts).

This study also provides new insights on how to deal with the scaling effect <u>e</u> problem when establishing <u>developing</u> large-large-scale <u>PM2.senvironmental variable (e.g. PM2.5 concentration)</u> prediction <u>mapping</u> models. <u>Instead ofRather than</u> ereating <u>constructing</u> a global model by gathering with all paired data <u>samples</u> into one <u>a single</u> training set, site-specific PM2.5 prediction models were firstly established using <u>a</u> random forest <u>model</u>, and <u>Follow that</u>, and a graph attention network was then <u>then applied developed</u> to establish an <u>ensemble learningspatial interpolation</u> model, <u>to integratinge multiple</u> on the basis of PM2.5 estimates derived from <u>site-specific</u> random forest models trained over sites with similar scene features as the target grid. By fully taking advantage of accounting for the scene similarity of between distant data samplegeographic regions, the proposed deep-learning methododel effectively attempted to Beeause Since there is no need to establish regional estimation models, <u>this</u> such a philosophy not only improves the modeling accuracy <u>andbut also</u> solve<u>address</u> the <u>sealing scale</u> problem in large-scale <u>PM2.5</u> modeling practices.

The LGHAP v2 dataset is publicly accessible <u>usingfrom</u> the <u>aforementioned</u> links <u>given above</u>. <u>The Given the merit of</u> <u>the gap-free and high-resolution merit, this dataset can be used to deepen our understanding of <u>be used as a reliable data source</u> <u>for assessing aerosol-aerosol-climatic climate effects interactions</u>, as well as PM_{2.5} exposure risks and related health outcomes at the global scalearound the world. <u>Also,Additionally</u>, the rResearchers are <u>also</u> encouraged to use this dataset to <u>better</u> evaluate the <u>status and trends of urban aerosol pollutions across the globe to support the assessment of sustainable Sustainable development <u>Development goals Goals-related to urban air quality across the globe</u>.</u></u>

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References

- Bai, K., and Li, K.: LGHAP: Long-term Gap-free High-resolution Air Pollutants concentration dataset, Zenodo [dataset], https://zenodo.org/communities/ecnu_lghap, 2023a.
- Bai, K., Chang, N.-B., and Chen, C.-F.: Spectral Information Adaptation and Synthesis Scheme for Merging Cross-Mission Ocean Color Reflectance Observations from MODIS and VIIRS, IEEE Transactions on Geoscience and Remote Sensing, 54, 311–329, https://doi.org/10.1109/TGRS.2015.2456906, 2016a.
- Bai, K., Chang, N.-B., Yu, H., and Gao, W.: Statistical bias correction for creating coherent total ozone record from OMI and OMPS observations, Remote Sensing of Environment, 182, 150–168, https://doi.org/10.1016/j.rse.2016.05.007, 2016b.
- Bai, K., Li, K., Chang, N.-B., and Gao, W.: Advancing the prediction accuracy of satellite-based PM2.5 concentration mapping: A perspective of data mining through in situ PM2.5 measurements, Environmental Pollution, 254, https://doi.org/10.1016/j.envpol.2019.113047, 2019.
- Bai, K., Li, K., Guo, J., and Chang, N.-B.: Multiscale and multisource data fusion for full-coverage PM2.5 concentration mapping: Can spatial pattern recognition come with modeling accuracy? ISPRS Journal of Photogrammetry and Remote Sensing, 184, 31–44, https://doi.org/10.1016/j.isprsjprs.2021.12.002, 2022b.
- Bai, K., Li, K., Guo, J., Yang, Y., and Chang, N.-B.: Filling the gaps of in situ hourly PM2.5 concentration data with the aid of empirical orthogonal function analysis constrained by diurnal cycles, Atmospheric Measurement Techniques, 13, 1213–1226, https://doi.org/10.5194/amt-13-1213-2020, 2020.
- Bai, K., Li, K., Ma, M., Li, K., Li, Z., Guo, J., Chang, N.-B., Tan, Z., and Han, D.: LGHAP: the Long-term Gap-free High-resolution Air Pollutant concentration dataset, derived via tensor-flow-based multimodal data fusion, Earth System Science Data, 14, 907–927, https://doi.org/10.5194/essd-14-907-2022, 2022a.
- Bai, K., Li, K., Sun, Y., Wu, L., Zhang, Y., Chang, N.-B., and Li, Z.: Global synthesis of two decades of research on improving PM2.5 estimation models from remote sensing and data science perspectives, Earth-Science Reviews, 241, 104461, https://doi.org/10.1016/j.earscirev.2023.104461, 2023b.

Beckers, J. M. and Rixen, M.: EOF calculations and data filling from incomplete oceanographic datasets, Journal Of Atmospheric And

Oceanic Technology, 20, 1839–1856, https://doi.org/10.1175/1520-0426(2003)020<1839:ECADFF>2.0.CO;2, 2003.

- Bi, J., Belle, J. H., Wang, Y., Lyapustin, A. I., Wildani, A., and Liu, Y.: Impacts of snow and cloud covers on satellite-derived PM2.5 levels, Remote Sensing of Environment, 221, 665–674, https://doi.org/10.1016/j.rse.2018.12.002, 2019.
- Buchard, V., Randles, C. A., da Silva, A. M., Darmenov, A., Colarco, P. R., Govindaraju, R., Ferrare, R., Hair, J., Beyersdorf, A. J., Ziemba, L. D., and Yu, H.: The MERRA-2 Aerosol Reanalysis, 1980 Onward. Part II: Evaluation and Case Studies, Journal of Climate, 30, 6851–6872, https://doi.org/10.1175/JCLI-D-16-0613.1, 2017.
- Burke, M., Childs, M. L., de la Cuesta, B., Qiu, M., Li, J., Gould, C. F., Heft-Neal, S., and Wara, M.: The contribution of wildfire to PM2.5 trends in the USA, Nature, 622, 761–766, https://doi.org/10.1038/s41586-023-06522-6, 2023.
- Che, H., Zhang, X.-Y., Xia, X., Goloub, P., Holben, B., Zhao, H., Wang, Y., Zhang, X.-C., Wang, H., Blarel, L., Damiri, B., Zhang, R., Deng, X., Ma, Y., Wang, T., Geng, F., Qi, B., Zhu, J., Yu, J., Chen, Q., and Shi, G.: Ground-based aerosol climatology of China: aerosol optical depths from the China Aerosol Remote Sensing Network (CARSNET) 2002–2013, Atmospheric Chemistry And Physics, 15, 7619– 7652, https://doi.org/10.5194/acp-15-7619-2015, 2015.
- Chen, X., Ding, J., Liu, J., Wang, J., Ge, X., Wang, R., and Zuo, H.: Validation and comparison of high-resolution MAIAC aerosol products over Central Asia, Atmospheric Environment, 251, 118273, https://doi.org/10.1016/j.atmosenv.2021.118273, 2021.
- Giles, D. M., Sinyuk, A., Sorokin, M. G., Schafer, J. S., Smirnov, A., Slutsker, I., Eck, T. F., Holben, B. N., Lewis, J. R., Campbell, J. R., Welton, E. J., Korkin, S. V., and Lyapustin, A. I.: Advancements in the Aerosol Robotic Network (AERONET) Version 3 database – automated near-real-time quality control algorithm with improved cloud screening for Sun photometer aerosol optical depth (AOD) measurements, Atmospheric Measurement Techniques, 12, 169–209, https://doi.org/10.5194/amt-12-169-2019, 2019.
- Guo, B., Wang, Z., Pei, L., Zhu, X., Chen, Q., Wu, H., Zhang, W., and Zhang, D.: Reconstructing MODIS aerosol optical depth and exploring dynamic and influential factors of AOD via random forest at the global scale, Atmospheric Environment, 315, 120159, https://doi.org/10.1016/j.atmosenv.2023.120159, 2023.
- Guo, J., Deng, M., Lee, S. S., Wang, F., Li, Z., Zhai, P., Liu, H., Lv, W., Yao, W., and Li, X.: Delaying precipitation and lightning by air pollution over the Pearl River Delta. Part I: Observational analyses, Journal of Geophysical Research: Atmospheres, 121, 6472–6488, https://doi.org/10.1002/2015JD023257, 2016.
- Guo, J., Su, T., Chen, D., Wang, J., Li, Z., Lv, Y., Guo, X., Liu, H., Cribb, M., and Zhai, P.: Declining summertime local-scale precipitation frequency over China and the United States, 1981–2012: The disparate roles of aerosols. Geophysical Research Letters, 46, 13281– 13289. https://doi.org/10.1029/2019GL085442, 2019.
- He, Q., Wang, W., Song, Y., Zhang, M., and Huang, B.: Spatiotemporal high-resolution imputation modeling of aerosol optical depth for investigating its full-coverage variation in China from 2003 to 2020, Atmospheric Research, 281, 106481, https://doi.org/10.1016/j.atmosres.2022.106481, 2023.
- Hersbach, H., Bell, B., Berrisford, P., Hirahara, S., Horányi, A., Muñoz-Sabater, J., Nicolas, J., Peubey, C., Radu, R., Schepers, D., Simmons, A., Soci, C., Abdalla, S., Abellan, X., Balsamo, G., Bechtold, P., Biavati, G., Bidlot, J., Bonavita, M., Chiara, G., Dahlgren, P., Dee, D., Diamantakis, M., Dragani, R., Flemming, J., Forbes, R., Fuentes, M., Geer, A., Haimberger, L., Healy, S., Hogan, R. J., Hólm, E., Janisková, M., Keeley, S., Laloyaux, P., Lopez, P., Lupu, C., Radnoti, G., Rosnay, P., Rozum, I., Vamborg, F., Villaume, S., and Thépaut, J.: The ERA5 global reanalysis, Quarterly Journal of the Royal Meteorological Society, 146, 1999–2049, https://doi.org/10.1002/qj.3803, 2020.
- Huang, X., Song, Y., Yang, J., Wang, W., Ren, H., Dong, M., Feng, Y., Yin, H., and Li, J.: Toward accurate mapping of 30-m time-series global impervious surface area (GISA), International Journal of Applied Earth Observation and Geoinformation, 109, 102787, https://doi.org/10.1016/j.jag.2022.102787, 2022.
- Jiang, J., Liu, J., Jiao, D., Zha, Y., and Cao, S.: Evaluation of MODIS DT, DB, and MAIAC Aerosol Products over Different Land Cover Types in the Yangtze River Delta of China, Remote Sensing (Basel), 15, 275, https://doi.org/10.3390/rs15010275, 2023.
- Johnson, J. M., Khoshgoftaar, T. M.: Survey on deep learning with class imbalance, Journal of Big Data, 6, 27. https://doi.org/10.1186/s40537-019-0192-5, 2019.
- Li, K., Bai, K., Jiao, P., Sun, Y., Shao, L., Li, X., Liu, C., Ma, M., Qiu, S., Zheng, Z., Han, D., Li, R., Li, Z., Guo, J., Chang, N.: SCAGAT: A scene-aware ensemble learning graph attention network for global PM2.5 pollution mapping, in preparation.
- Li, K., Bai, K., Li, Z., Guo, J., and Chang, N.-B.: Synergistic data fusion of multimodal AOD and air quality data for near real-time full coverage air pollution assessment, Journal of Environmental Management, 302, 114121, https://doi.org/10.1016/j.jenvman.2021.114121, 2022b.
- Li, K., Bai, K., Ma, M., Guo, J., Li, Z., Wang, G., and Chang, N.-B.: Spatially gap free analysis of aerosol type grids in China: First retrieval via satellite remote sensing and big data analytics, ISPRS Journal of Photogrammetry and Remote Sensing, 193, 45–59, https://doi.org/10.1016/j.isprsjprs.2022.09.001, 2022a.
- Li, L., Franklin, M., Girguis, M., Lurmann, F., Wu, J., Pavlovic, N., Breton, C., Gilliland, F., and Habre, R.: Spatiotemporal imputation of MAIAC AOD using deep learning with downscaling, Remote Sensing of Environment, 237, 111584, https://doi.org/10.1016/j.rse.2019.111584, 2020.
- Li, Z. Q., Xu, H., Li, K. T., Li, D. H., Xie, Y. S., Li, L., Zhang, Y., Gu, X. F., Zhao, W., Tian, Q. J., Deng, R. R., Su, X. L., Huang, B., Qiao, Y. L., Cui, W. Y., Hu, Y., Gong, C. L., Wang, Y. Q., Wang, X. F., Wang, J. P., Du, W. B., Pan, Z. Q., Li, Z. Z., and Bu, D.: Comprehensive study of optical, physical, chemical, and radiative properties of total columnar atmospheric aerosols over China: An overview of sun– Sky radiometer observation network (SONET) measurements, Bulletin of the American Meteorological Society, 99, 739–755, https://doi.org/10.1175/BAMS-D-17-0133.1, 2018.
- Li, Z., Guo, J., Ding, A., Liao, H., Liu, J., Sun, Y., Wang, T., Xue, H., Zhang, H., and Zhu, B.: Aerosol and boundary-layer interactions and impact on air quality, National Science Review, 4, 810–833, https://doi.org/10.1093/nsr/nwx117, 2017.
- Li, Z., Wang, Y., Guo, J., Zhao, C., Cribb, M. C., Dong, X., Fan, J., Gong, D., Huang, J., Jiang, M., Jiang, Y., Lee, S. S., Li, H., Li, J., Liu, J., Qian, Y., Rosenfeld, D., Shan, S., Sun, Y., Wang, H., Xin, J., Yan, X., Yang, X., Yang, X., Zhang, F., and Zheng, Y.: East Asian Study of Tropospheric Aerosols and their Impact on Regional Clouds, Precipitation, and Climate (EAST-AIRCPC), Journal of Geophysical Research: Atmospheres, 124, 13026–13054, https://doi.org/10.1029/2019JD030758, 2019.
- Liang, F., Xiao, Q., Huang, K., Yang, X., Liu, F., Li, J., Lu, X., Liu, Y., and Gu, D.: The 17-y spatiotemporal trend of PM2.5 and its mortality

burden in China, Proceedings of the National Academy of Sciences, 117, 25601–25608, https://doi.org/10.1073/pnas.1919641117, 2020. Liu, J., Ren, C., Huang, X., Nie, W., Wang, J., Sun, P., Chi, X., and Ding, A.: Increased Aerosol Extinction Efficiency Hinders Visibility

- Improvement in Eastern China, Geophysical Research Letters, 47, https://doi.org/10.1029/2020GL090167, 2020.
- Liu, N., Zou, B., Feng, H., Wang, W., Tang, Y., and Liang, Y.: Evaluation and comparison of multiangle implementation of the atmospheric correction algorithm, Dark Target, and Deep Blue aerosol products over China, Atmospheric Chemistry and Physics, 19, 8243–8268, https://doi.org/10.5194/acp-19-8243-2019, 2019.
- Liu, X. and Wang, M.: Filling the gaps of missing data in the merged VIIRS SNPP/NOAA-20 ocean color product using the DINEOF method, Remote Sensing (Basel), 11, https://doi.org/10.3390/rs11020178, 2019.
- Lyapustin, A., Wang, Y., Korkin, S., and Huang, D.: MODIS Collection 6 MAIAC algorithm, Atmospheric Measurement Techniques, 11, 5741–5765, https://doi.org/10.5194/amt-11-5741-2018, 2018.
- Lyapustin, A., Wang, Y., Laszlo, I., Kahn, R., Korkin, S., Remer, L., Levy, R., and Reid, J. S.: Multiangle implementation of atmospheric correction (MAIAC): 2. Aerosol algorithm, Journal of Geophysical Research Atmospheres, 116, 1–15, https://doi.org/10.1029/2010JD014986, 2011.
- Ma, Z., Liu, Y., Zhao, Q., Liu, M., Zhou, Y., and Bi, J.: Satellite-derived high resolution PM2.5 concentrations in Yangtze River Delta Region of China using improved linear mixed effects model, Atmospheric Environment, 133, 156–164, https://doi.org/10.1016/j.atmosenv.2016.03.040, 2016.
- Martins, V. S., Lyapustin, A., Carvalho, L. A. S., Barbosa, C. C. F., and Novo, E. M. L. M.: Validation of high-resolution MAIAC aerosol product over South America, Journal of Geophysical Research: Atmospheres, 122, 7537–7559, https://doi.org/10.1002/2016JD026301, 2017.
- Mhawish, A., Banerjee, T., Sorek-Hamer, M., Lyapustin, A., Broday, D. M., and Chatfield, R.: Comparison and evaluation of MODIS Multiangle Implementation of Atmospheric Correction (MAIAC) aerosol product over South Asia, Remote Sensing of Environment, 224, 12–28, https://doi.org/10.1016/j.rse.2019.01.033, 2019.
- Qin, W., Fang, H., Wang, L., Wei, J., Zhang, M., Su, X., Bilal, M., and Liang, X.: MODIS high-resolution MAIAC aerosol product: Global validation and analysis, Atmospheric Environment, 264, 118684, https://doi.org/10.1016/j.atmosenv.2021.118684, 2021.
- Randles, C. A., da Silva, A. M., Buchard, V., Colarco, P. R., Darmenov, A., Govindaraju, R., Smirnov, A., Holben, B., Ferrare, R., Hair, J., Shinozuka, Y., and Flynn, C. J.: The MERRA-2 Aerosol Reanalysis, 1980 Onward. Part I: System Description and Data Assimilation Evaluation, Journal of Climate, 30, 6823–6850, https://doi.org/10.1175/JCLI-D-16-0609.1, 2017.
- Shannon, C. E.: A Mathematical Theory of Communication, Bell System Technical Journal, 27, 379–423, 1948.
- Shi, H., Zhang, Y., Chen, Y., Ji, S., Dong, Y.: Resampling algorithms based on sample concatenation for imbalance learning, Knowledge-Based Systems, 245, 108592. https://doi.org/10.1016/j.knosys.2022.108592, 2022.
- Sogacheva, L., Popp, T., Sayer, A. M., Dubovik, O., Garay, M. J., Heckel, A., Christina Hsu, N., Jethva, H., Kahn, R. A., Kolmonen, P., Kosmale, M., De Leeuw, G., Levy, R. C., Litvinov, P., Lyapustin, A., North, P., Torres, O., and Arola, A.: Merging regional and global aerosol optical depth records from major available satellite products, Atmospheric Chemistry and Physics, 20, 2031–2056, https://doi.org/10.5194/acp-20-2031-2020, 2020.
- Tang, Q., Bo, Y., and Zhu, Y.: Spatiotemporal fusion of multiple-satellite aerosol optical depth (AOD) products using Bayesian maximum entropy method, Journal of Geophysical Research: Atmospheres, 121, 4034–4048, https://doi.org/10.1002/2015JD024571, 2016.
- Up in the aerosol, Nature Geoscience, 15, 157, https://doi.org/10.1038/s41561-022-00915-4, 2022.
- Wang, Y. W. and Yang, Y. H.: China's dimming and brightening: Evidence, causes and hydrological implications, Annales Geophysicae, 32, 41–55, https://doi.org/10.5194/ANGEO-32-41-2014, 2014.
- Wang, Y., Yuan, Q., Zhou, S., and Zhang, L.: Global spatiotemporal completion of daily high-resolution TCCO from TROPOMI over land using a swath-based local ensemble learning method, ISPRS Journal of Photogrammetry and Remote Sensing, 194, 167–180, https://doi.org/10.1016/j.isprsjprs.2022.10.012, 2022.
- Wei, J., Li, Z., Lyapustin, A., Sun, L., Peng, Y., Xue, W., Su, T., and Cribb, M.: Reconstructing 1-km-resolution high-quality PM2.5 data records from 2000 to 2018 in China: spatiotemporal variations and policy implications, Remote Sensing of Environment, 252, 112136, https://doi.org/10.1016/j.rse.2020.112136, 2021a.
- Wei, X., Bai, K., Chang, N.-B., and Gao, W.: Multisource hierarchical data fusion for high-resolution AOD mapping in a forest fire event, International Journal of Applied Earth Observation and Geoinformation, 102, 102366, https://doi.org/10.1016/j.jag.2021.102366, 2021b.
- Wei, X., Chang, N.-B., Bai, K., and Gao, W.: Satellite remote sensing of aerosol optical depth: advances, challenges, and perspectives, Critical Reviews in Environmental Science and Technology, 50, 1640–1725, https://doi.org/10.1080/10643389.2019.1665944, 2020.
 WHO: Ambient air pollution, 2022.
- Wild, M., Wacker, S., Yang, S., and Sanchez-Lorenzo, A.: Evidence for Clear-Sky Dimming and Brightening in Central Europe, Geophysical Research Letters, 48, https://doi.org/10.1029/2020GL092216, 2021.
- Xiao, Q., Geng, G., Cheng, J., Liang, F., Li, R., Meng, X., Xue, T., Huang, X., Kan, H., Zhang, Q., and He, K.: Evaluation of gap-filling approaches in satellite-based daily PM2.5 prediction models, Atmospheric Environment, 244, 117921, https://doi.org/10.1016/j.atmosenv.2020.117921, 2021.
- Xiao, Q., Wang, Y., Chang, H. H., Meng, X., Geng, G., Lyapustin, A., and Liu, Y.: Full-coverage high-resolution daily PM2.5 estimation using MAIAC AOD in the Yangtze River Delta of China, Remote Sensing of Environment, 199, 437–446, https://doi.org/10.1016/j.rse.2017.07.023, 2017.
- Xu, H., Guang, J., Xue, Y., de Leeuw, G., Che, Y. H., Guo, J., He, X. W., and Wang, T. K.: A consistent aerosol optical depth (AOD) dataset over mainland China by integration of several AOD products, Atmospheric Environment, 114, 48–56, https://doi.org/10.1016/j.atmosenv.2015.05.023, 2015.
- Yang, X., Zhao, C., Zhou, L., Wang, Y., and Liu, X.: Distinct impact of different types of aerosols on surface solar radiation in China, Journal of Geophysical Research: Atmospheres, 121, 6459–6471, https://doi.org/10.1002/2016JD024938, 2016.
- Yang, Y., Ren, L., Li, H., Wang, H., Wang, P., Chen, L., Yue, X., and Liao, H.: Fast Climate Responses to Aerosol Emission Reductions During the COVID-19 Pandemic, Geophysical Research Letters, 47, https://doi.org/10.1029/2020GL089788, 2020.
- Zhang, Q., Zheng, Y., Tong, D., Shao, M., Wang, S., Zhang, Y., Xu, X., Wang, J., He, H., Liu, W., Ding, Y., Lei, Y., Li, J., Wang, Z., Zhang,

X., Wang, Y., Cheng, J., Liu, Y., Shi, Q., Yan, L., Geng, G., Hong, C., Li, M., Liu, F., Zheng, B., Cao, J., Ding, A., Gao, J., Fu, Q., Huo, J., Liu, B., Liu, Z., Yang, F., He, K., and Hao, J.: Drivers of improved PM2.5 air quality in China from 2013 to 2017, Proceedings of the National Academy of Sciences of the United States of America, 116, 24463–24469, https://doi.org/10.1073/pnas.1907956116, 2019.
Zhang, T., Zhou, Y., Zhao, K., Zhu, Z., Asrar, G. R., and Zhao, X.: Gap-filling MODIS daily aerosol optical depth products by developing a spatiotemporal fitting algorithm, Giscience & Remote Sensing, 59, 762–781, https://doi.org/10.1080/15481603.2022.2060596, 2022.
Zhao, C., Yang, Y., Fan, H., Huang, J., Fu, Y., Zhang, X., Kang, S., Cong, Z., Letu, H., and Menenti, M.: Aerosol characteristics and impacts

on weather and climate over the Tibetan Plateau, National Science Review, 7, 492–495, https://doi.org/10.1093/nsr/nwz184, 2020.