Vertical Retrieval of AOD using SEVIRI data, Case Study: European Continent

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Abstract. Accurately determining Aerosol Optical Depth (AOD) across various altitudes with sufficient spatial and temporal resolution is crucial for effective aerosol monitoring, given the significant variations over time and space. While ground-based observations provide detailed vertical profiles, satellite data are crucial for addressing spatial and temporal gaps. This study utilizes profiles from the Cloud-Aerosol Lidar with Orthogonal Polarization (CALIOP) and data from the Spinning Enhanced Visible and Infrared Imager (SEVIRI) to estimate vertical AOD values at 1.5, 3, 5, and 10 km layers. These estimations are achieved with spatial and temporal resolutions of 3 km × 3 km and 15 minutes, respectively, over Europe. We employed machine learning models—XGBoost (XGB) and Random Forest (RF)—trained on SEVIRI data from 2017 to 2019 for the estimations. Validation using CALIOP AOD retrievals in 2020 confirmed the reliability of our findings, emphasizing the importance of wind speed (Ws) and wind direction (Wd) in improving AOD estimation accuracy. A comparison between seasonal and annual models revealed slight variations in accuracy, leading to the selection of annual models as the preferred approach for estimating SEVIRI AOD profiles. Among the annual models, the RF model demonstrated superior performance over the XGB model at higher layers, yielding more reliable AOD estimations. Further validation using data from EARLINET stations across Europe in 2020 indicated that the XGB model achieved better agreement with EARLINET AOD profiles, with $R^2$ values of 0.81, 0.77, 0.71, and 0.56, and RMSE values of 0.03, 0.01, 0.02, and 0.005, respectively.

Keywords: AOD Vertical Profile, SEVIRI, Geostationary satellite, CALIOP, EARLINET, Machine Learning.

1 Introduction

Researchers acknowledge that aerosols significantly contribute to air pollution, climate change, and alterations in solar and thermal infrared radiation absorption and scattering (Hyslop, 2009; Pope et al., 2019; Li et al., 2022). Understanding their behaviour is crucial for refining atmospheric models and monitoring techniques. Aerosol Optical Depth (AOD) serves as a parameter for quantitatively estimating both the aerosol concentration and its optical properties. Recent researches highlight the pivotal role of aerosol vertical profiles in AOD retrieval uncertainties (Wang et al., 2018, Rogozovsky et al., 2021; Gupta et al., 2021; Rogozovsky et al., 2023). Moreover, understanding the vertical layering of aerosol properties enhances insights
into aerosol transport mechanisms, aids in source identification, elucidates atmospheric dynamics, and improves the accuracy of models tracking long-range aerosol transport (Chen et al., 2023). Consequently, continuous monitoring of the large-scale three-dimensional properties of aerosols in the atmosphere remains imperative.

Vertical AOD retrieval can be conducted through ground-based observations or inferred from remote sensing data. Ground-based LiDAR networks, such as the European Aerosol Research Lidar Network (EARLINET), provide detailed insights into various aerosol properties by offering vertical profiles of aerosol optical properties (Bösenberg et al., 2001, 2003). While these observations offer detailed vertical information, their sparse nature necessitates supplementation with satellite observations.

Satellite remote sensing emerges as the primary method for capturing temporal and spatial variations in aerosol profiles globally. While passive satellite remote sensing significantly enhances spatial coverage for aerosol monitoring, it lacks the detailed resolution of aerosol vertical layers provided by active techniques (Hsu et al., 2004; Levy et al., 2013). Spaceborne LiDAR systems, such as the Cloud-Aerosol Lidar with Orthogonal Polarization (CALIOP) onboard the Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observation (CALIPSO) satellite launched in 2006, offer distributions of aerosols and clouds, along with their geometrical and optical properties. The CALIOP instrument represents the world's first operational satellite-based cloud and aerosol LiDAR (Winker et al., 2004, 2006), providing high-resolution global aerosol vertical profile data that facilitate vertical distribution studies (Winker et al., 2007). However, the CALIOP sensor encounters challenges in achieving adequate spatial and temporal coverage, with limitations in daily and global resolution (16-day temporal resolution and 5 km profile distance).

To address the limitations related to the inadequate spatial and temporal coverage of CALIOP, recent studies by Pashayi et al. (2023, 2024) have introduced Seasonal and Seasonal-Independent models. These models seek to investigate the relationship between MODIS observations, MAIAC, and CALIOP AOD for Vertical Layering of MAIAC AOD product at a spatial-temporal resolution corresponding to the MAIAC product, with a focus on the Persian Gulf region. The researchers subsequently analyse their findings using CALIOP AOD retrievals across distinct vertical layers. Despite promising outcomes, the temporal variability and transient lifespan of aerosols, particularly within vertical layers, pose challenges to the effectiveness of estimated AOD products in these studies. This limitation stems from the utilization of MODIS products aboard polar-orbiting satellites, which pass over a region approximately once a day during daylight hours, thus inadequately supporting aerosol monitoring at high temporal resolution (Wei et al., 2020).

Geostationary satellites provide observations with significantly high temporal resolutions (Wei et al., 2020). In recent years, numerous geostationary satellite sensors with enhanced radiometric, spectral, and spatial resolutions have been deployed to monitor global aerosol loading with temporal resolutions of less than an hour. Notable examples of these geostationary sensors include Himawari-8, equipped with the Advanced Himawari Imager (AHI, Da, 2015); the Advanced Baseline Imager (ABI, Kalluri et al., 2015) aboard the Geostationary Operational Environmental Satellite (GOES); and the Meteosat geostationary satellites, equipped with the Spinning Enhanced Visible and Infrared Imager (SEVIRI, Pasternak et al., 1994) instrument. These advancements facilitate observations with high temporal resolution, substantially enhancing aerosol monitoring capabilities across various regions (Schmit et al., 2018; Zhang et al., 2019; Ge et al., 2019; Tang et al., 2019; Zawadzka-Manko...
et al., 2020; Witthuhn et al., 2020; Kocaman et al., 2022; Ceamanos et al., 2023). Specifically, SEVIRI offers suitable temporal and spatial resolutions, presenting a valuable opportunity to expand aerosol datasets for Europe (Stebel et al., 2021; Nicolae et al., 2021).

The retrieval of AOD values typically entails two primary approaches: physically based methods (Seidel et al., 2012; Lipponen et al., 2018; Amini et al., 2021; Mehta et al., 2022) and data mining techniques (Radosavljevic et al., 2010; She et al., 2020; Chen et al., 2022). Physically based methods rely on established principles of aerosol behaviour, utilizing models derived from physical laws to estimate AOD values. However, these methods encounter limitations due to uncertainties in inputs and the complex nature of particle phenomena. In contrast, data mining techniques offer a promising alternative by harnessing large datasets and employing machine learning algorithms to discern patterns and relationships within complex aerosol systems.

In this study, our objective is to introduce a model for enhancing the temporal resolution of AOD profile products over Europe continent by integrating SEVIRI-based information with CALIOP aerosol profile products. To achieve this, we develop a machine learning (ML) model capable of retrieving sub-hourly (approximately every 15 minutes) vertical AOD values with a spatial resolution of 3 km × 3 km. Leveraging two well-established ML models—XGBoost (XGB) and Random Forest (RF)—previously demonstrated effective in similar studies, these algorithms serve as the foundation for training layering models and assessing their seasonal independence using numerical datasets. Importantly, previous studies (Zhang et al., 2021; Lebo, 2014; Marinescu et al., 2017) have demonstrated that aerosols situated in the mid-troposphere (at altitudes ranging from 3 to 10 kilometres) significantly influence cloud characteristics (Lebo, 2014), while those in the lower troposphere have a pronounced effect on mixed-phase precipitation (Marinescu et al., 2017). Consequently, our focus is on developing region-specific models to estimate AOD values across the 1.5, 3, 5, and 10 km layers for each pixel of the SEVIRI dataset, thus notably improving the spatial-temporal resolution of AOD in these layers. Furthermore, the existence of EARLINET stations across Europe aims to validate the estimated AOD values. We organized the rest of the paper as follows: Section 2 provides a comprehensive overview of the dataset employed, while Section 3 details the necessary pre-processing steps and retrieval methodology. Subsequently, Section 4 delves into the discussion of the vertically retrieved AOD results, followed by conclusions outlined in Section 5.

2 Study Area and Data Source

2.1 Study Area

The study area encompasses a significant portion of Europe, spanning from 35°N to 71°N and -7°E to 70°E, covering approximately 10.18 million square kilometres. Despite its relatively small land area, Europe exhibits a diverse geographical landscape and complex atmospheric dynamics. Urban centers in Europe face persistent air pollution issues due to industrial activities and vehicular emissions, compounded by the effects of climate change. Various aerosol types, originating from industrial processes, transportation, biomass burning, and natural events significantly impact air quality, weather patterns, and climate dynamics across the continent. Long-range transport of aerosols, particularly from sources in Africa such as Saharan
dust storms, underscores the interconnectedness of atmospheric processes across continents and emphasizes the necessity of international cooperation in addressing air pollution and environmental challenges.

2.2 Data Source

2.2.1 SEVIRI

The Meteosat Second Generation (MSG) constitutes a series of four satellites managed by the Exploitation of Meteorological Satellites (EUMETSAT) and has been operational since 2004. Originally designated as MSG1 to MSG4, these satellites were subsequently rebranded as Meteosat-8 to Meteosat-11, respectively. The primary instrument onboard these satellites is the Spinning Enhanced Visible and Infrared Imager (SEVIRI), a radiometer equipped with 11 spectral channels spanning the visible to the infrared spectrum. SEVIRI provides a spatial resolution of 3 km at the sub-satellite point, with a high-resolution visible (HRV) channel offering a spatial resolution of 1 km at nadir. Strategically centered at various wavelengths, the thermal channels of SEVIRI include 6.2 and 7.3 µm (targeting strong water vapor absorption), 8.7, 10.8, and 12.0 µm (window channels), as well as 9.7 µm (for ozone absorption) and 13.4 µm (for carbon dioxide absorption). This operational system delivers full-disk Earth data, while the rapid scan service focuses on observing the upper part of the Earth's disk, covering Europe and North Africa, with a repetition time of 15 minutes (Schmetz et al., 2002; Zawadzka et al., 2014). In our study, we primarily utilize SEVIRI data from Meteosat-11, the fourth and final flight unit of the MSG program, which was launched on July 15, 2015. Meteosat-11 currently operates in geostationary orbit, positioned at 36,000 km above the equator. Its coverage extends over Europe, Africa, and the Indian Ocean, spanning from -81 to 81 degrees longitude and -79 to 79 degrees latitude. Figure 1 provides a visualization of the coverage area of SEVIRI.

Figure 1. The area covered by the SEVIRI instrument (https://data.eumetsat.int/data/map/EO:EUM:DAT:MSG:HRSEVIRI).
2.2.2 CALIOP

The CALIOP instrument plays a pivotal role in the CALIPSO satellite, launched in April 2006 with the primary objective of reliably delivering high-resolution vertical profiles of global aerosol properties via an active sensing technique. Functioning as a polarization-sensitive LiDAR, CALIOP measures the depolarization ratio, serving as a degree of particle irregularity. CALIOP is specifically designed to observe aerosol optical properties during both the day and night, focusing on vertical layers at wavelengths of 532 and 1064 nm. Its Level 2 algorithm not only provides information on aerosol optical characteristics like particle depolarization ratio and color ratio but also retrieves extinction coefficients. Notably, CALIOP data offer a temporal resolution of approximately 16 days, capturing insights into aerosol dynamics over time. Sampling occurs at intervals of 333 m along the orbital track, maintaining a vertical resolution of 60 m from altitudes of 0.5 to 20 km and 180 m from 20 to 30 km within the vertical profile (Winker et al., 2004, 2006, and 2007). For this study, we employed CALIOP level 2 Version 4.2 aerosol profile products, featuring a horizontal resolution of 5 km and a vertical resolution of 60 m up to an altitude of 20.2 km. These data, spanning from 2017 to 2019, were utilized to estimate the profiles of AOD at layers of 1.5, 3, 5, and 10 km (denoted as $AOD_{1.5}$, $AOD_3$, $AOD_5$, and $AOD_{10}$) within the defined study region.

2.2.3 MODIS land cover data

In this research, we leveraged land cover data spanning 2017 to 2019, with a spatial resolution of 1 km, sourced from the global MODIS products (MCD12Q1 V6) covering Europe. These data, derived from both Terra and Aqua satellites, provide comprehensive land cover types annually from 2001. The dataset encompasses six classification schemes, elucidated in the downloadable User Guide available at https://ladsweb.modaps.eosdis.nasa.gov/. Each MCD12Q1 Version 6 Hierarchical Data Format 4 (HDF4) file comprises layers for Land Cover Type 1-5, Land Cover Property 1-3, Land Cover Property Assessment 1-3, Land Cover Quality Control (QC), and a Land Water Mask (Sulla-Menashe and Friedl, 2018). Our study specifically focuses on the first classification scheme, the Annual International Geosphere-Biosphere Program (IGBP) classification.

2.2.4 Meteorological data

Meteorological data were acquired from the European Centre for Medium-Range Weather Forecasts (ECMWF) dataset, accessible at (https://cds.climate.copernicus.eu/). ECMWF has been actively operational in real-time seasonal forecast systems since 1997, providing access to standard meteorological data. This dataset comprises two distinct sets of data (Copernicus Climate Change Service, Climate Data Store, (2021)). Firstly, version 2 of the Integrated Global Radiosonde Archive (IGRA) from 1978 integrates global radio sounding containing temperature, humidity, and wind data from various sources. The dataset is presented in the form of a global grid with a conventional grid resolution of $0.25^\circ \times 0.25^\circ$. Compared with previous-generation products, the temporal resolution has been increased from 6 hours to 1 hour, enabling the study of diurnal variations in the troposphere. Secondly, the Radio Sounding HARMonization (RHARM) homogenized dataset offers adjusted values for temperature, relative humidity, and wind. RHARM effectively eliminates systematic effects such as variations in measurement.
sensors, biases induced by solar radiation, calibration drifts, station relocations, and other factors, across 700 IGRA radiosonde stations and ship-based radio soundings. RHARM includes twice-daily (0000 and 1200 UTC) radiosonde data at mandatory and standard levels, featuring essential parameters like air temperature (T, K), air pressure (P, Pa), wind speed (Ws, m/s), and wind direction (Wd, degrees from north). For this study, the global grid dataset is utilized over the European continent from 2017 to 2019, as depicted in Fig. 2.

Figure 2. Map depicting the ECMWF stations for meteorological data measurements (Durre et al., 2016).

2.2.5 EARLINET

EARLINET, established in the year 2000 (Bösenberg et al., 2001, 2003), originated as a research project funded by the European Commission within the framework of the Fifth Framework Program. The primary objective of EARLINET is to generate profiles of aerosol optical properties, thereby constructing an expansive, quantitative, and statistically robust database for the continental-scale distribution of aerosols. This initiative aims to enhance network operations, facilitate research on aerosol-related processes, validate satellite sensor data, advance model development and validation, integrate aerosol data into operational models, and compile a comprehensive climatology of aerosol distribution. Currently, the network comprises 30 active stations, with the majority equipped with Raman LiDAR featuring depolarization channels. These Raman LiDAR-operating EARLINET stations typically provide profiles of aerosol extinction and backscatter coefficients without relying on significant assumptions. Figure 3 illustrates the distribution of EARLINET stations over the study area.
3 Methodology

In this paper, our primary objective is to establish a robust relationship between the input variables—SEVIRI band measurements, meteorological data, and land cover products—and the vertical AOD profiles at 1.5, 3, 5, and 10 km layers. To identify this relationship, we use CALIOP AOD retrievals at these layers as reference data. Our proposed model framework for estimating AOD at the four distinct layers encompasses several sequential steps: data collection, preprocessing, partitioning, regression, and analysis of the performance of each regression model to ascertain the most accurate one, as illustrated in Fig. 4.

The process commences with data collection, detailed in the preceding section. Subsequently, preprocessing of both input and output data becomes imperative to ensure their suitability for subsequent analysis. The dataset is then partitioned into two subsets: training and testing, a pivotal step in ML aimed at assessing model performance and mitigating overfitting. Following data partitioning, various ML model structures are proposed and developed to capture the intricate relationships within the dataset. This phase entails selecting appropriate algorithms and architectures tailored to the specific task of AOD estimation. Finally, the performance of each model is meticulously evaluated using predefined metrics to pinpoint the most accurate and
A reliable model for AOD estimation across the desired vertical layers. In the subsequent sections, we will delve into a detailed examination of each step.

Figure 4. Research framework for developing ML models to estimate SEVIRI AOD profiles.
3.1 Pre-Processing

To ensure a robust model for estimating AOD values at suitable 3D resolutions, this study integrates data from various sources, including satellites and ground-based observations. To address spatial-temporal sampling disparities, we employ a co-location approach where data from multiple sources, such as satellites and ground-based observations, are matched within a ±30 minutes timeframe and within a 3 km radius of the study area (Kittaka et al., 2011; Redemann et al., 2012; Han et al., 2017; Liu et al., 2018a). This method harmonizes disparate datasets, enhancing the reliability and comprehensiveness of our analysis. The subsequent preprocessing stages necessary for data refinement and analysis are elaborated upon in the following subsections.

3.1.1 SEVIRI

Utilizing SEVIRI data necessitates a critical preprocessing step involving co-referencing and applying geometric corrections. The Data Tailor tool, accessible at https://www.eumetsat.int/data-tailor, serves as a valuable spatial resource introduced in recent years. It simplifies the definition of coordinate systems, image systems, cutting ranges, expected output types, and requisite file extensions for the output data. Estimating AOD values requires the conversion of radiance to reflectance for the SEVIRI reflective bands (VIS06, VIS08, and NIR16), and equivalent brightness temperature for the remaining eight bands. To achieve this, we computed the Bidirectional Reflectance Factor (BRF) for the SEVIRI warm channels using Equation (1) proposed by the European Organization for the Exploitation of Meteorological Satellites (2012):

\[
r_{\lambda_i} = \frac{\pi R_{\lambda_i} d^2(t)}{I_{\lambda_i} \cos(\theta(t,x))},
\]

where \(i\) denotes the channel number (1 = VIS06, 2 = VIS08, 3 = NIR16, 4 = HRV), \(r_{\lambda_i}\) represents the Bidirectional Reflectance Factor (BRF) for channel \(\lambda_i\), \(R_{\lambda_i}\) stands for the measured radiance in mW·m\(^{-2}\)·sr\(^{-1}\)·(cm\(^{-1}\))\(^{-1}\), \(d(t)\) signifies the Sun-Earth distance in Astronomical Unit (AU) at time \(t\), \(I_{\lambda_i}\) signifies the band solar irradiance for channel \(\lambda_i\) at 1 AU in mW·m\(^{-2}\)·sr\(^{-1}\)·(cm\(^{-1}\))\(^{-1}\), and \(\theta(t, x)\) denotes the Solar Zenith Angle in radians at time \(t\) and location \(x\). The equivalent brightness temperature \((T_b)\) of a satellite observation is defined as the temperature of a black body emitting the same amount of radiation. Therefore, the brightness temperature follows the form of Equation (2).

\[
T_b = \frac{c_2 v_c}{a \log(c_1 v_e^2/R + 1)} - \frac{\beta}{\alpha},
\]

Using the observed radiances \(\bar{R}\) (in mW m\(^{-2}\) sr\(^{-1}\) (cm\(^{-1}\))\(^{-1}\)) and radiation constants \(C_1 = 2hc^3\) and \(C_2 = hc/k\), where \(c\), \(h\), and \(k\) represent the speed of light, Planck’s constant, and the Boltzmann constant respectively, the regression coefficients \(v_e\), \(\alpha\), and \(\beta\) are determined through non-linear regression analysis. This analysis is conducted on a pre-calculated lookup table generated for the various SEVIRI channels, as delineated in Table 1 (Tjemkes et al., 2012).
Table 1. Values for the regression parameters.

<table>
<thead>
<tr>
<th>Channel No.</th>
<th>Channel ID</th>
<th>$v_c, cm^{-1}$</th>
<th>$\alpha$</th>
<th>$\beta, K$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>IR 3.9</td>
<td>2567.330</td>
<td>0.9956</td>
<td>3.410</td>
</tr>
<tr>
<td>5</td>
<td>WV 6.2</td>
<td>1598.103</td>
<td>0.9962</td>
<td>2.218</td>
</tr>
<tr>
<td>6</td>
<td>WV 7.3</td>
<td>1362.081</td>
<td>0.9991</td>
<td>0.478</td>
</tr>
<tr>
<td>7</td>
<td>IR 8.7</td>
<td>1149.069</td>
<td>0.9996</td>
<td>0.179</td>
</tr>
<tr>
<td>8</td>
<td>IR 9.7</td>
<td>1034.343</td>
<td>0.9999</td>
<td>0.060</td>
</tr>
<tr>
<td>9</td>
<td>IR 10.8</td>
<td>930.647</td>
<td>0.9983</td>
<td>0.625</td>
</tr>
<tr>
<td>10</td>
<td>IR 12.0</td>
<td>839.660</td>
<td>0.9988</td>
<td>0.397</td>
</tr>
<tr>
<td>11</td>
<td>IR 13.4</td>
<td>752.387</td>
<td>0.9981</td>
<td>0.578</td>
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</table>

3.1.2 CALIOP

In this study, to mitigate the impact of cloud contamination and retrieval errors on CALIOP AOD retrieval, our screening methods closely follow the guidelines established by Winker et al., 2013. We employ various quality filters to identify and filter aerosol pixels, including CAD scores, extinction QC flags, and uncertainty values. Specifically, we utilize a CAD score range outside [-100, -20] to address uncertainties in cloud-aerosol discrimination, ensuring the selection of cloud-free pixels with high confidence. Additionally, we apply extinction quality control flags with values 0 and 1 to filter extinction retrievals with high confidence. This includes constrained retrievals utilizing transmittance measurements and unconstrained retrievals where the initial LiDAR ratio remains unchanged in iterations. Furthermore, we exclusively consider daytime profiles in this study. Uncertainty flags associated with extinction coefficients are employed for data screening. Range bins with an uncertainty flag value of 99.9 km$^{-1}$ are excluded from the analysis, following the methodology outlined by Winker et al., 2013.

3.1.3 Land Cover Product

Considering that the original MCD12Q1 product is stored in a HDF and utilizes the sinusoidal projection, several data preprocessing steps are required. These steps encompass format conversion, reprojection, resampling, image mosaicking, and sub-area masking. To execute these tasks, we employ the pyModis Free and Open-Source Python-based library. This tool enables the conversion of MODIS HDF data format into Geotiff format and facilitates the conversion of data projection from SIN to WGS84/UTM. Additionally, it facilitates image mosaicking and sub setting. Moreover, to enable comparison between the MCD12Q1 and SEVIRI datasets, the spatial resolution of MCD12Q1 is resampled at 3 km using the nearest neighbor resampling method. This method preserves the gray values of the original image, unlike bilinear interpolation or cubic convolution interpolation methods, which may alter them.
3.2 ML Models and parameter Tuning

In this study, our primary objective is to develop a ML model to estimate SEVIRI AOD values at various altitudes—1.5 km, 3 km, 5 km, and 10 km—using CALIOP’s vertical profiles across the European continent. We employ two distinct ML algorithms, RF and XGBoost, to train layering models. Both RF and XGBoost adopt an ensemble approach, which involves constructing and aggregating multiple decision trees (Breiman, 2001; Chen and Guestrin, 2016). In RF, each tree is built using a bootstrap sample of the data, with nodes determined by the best subset of randomly selected predictors (Breiman, 2001). These trees are then averaged to obtain a final ensemble prediction. Conversely, XGBoost implements the gradient boosting method, where trees are interdependent as newly trained trees are constructed based on previous trees, incorporating their ability to predict the residuals of prior trees (Chen and Guestrin, 2016). In both RF and XGBoost, all trained trees are combined to make the final prediction.

We systematically explored various parameter combinations for each ML model. Parameters such as the number of decision trees (N_estimators), the number of variables considered for splitting at each node (max_features), and the maximum depth of each decision tree (max_depth) for RF, as well as parameters including the number of gradient boosting rounds or decision trees (n_estimators), minimum sum of instance weight (Min_sample_split), maximum depth of each decision tree (max_depth), and minimum number of samples required to be at a leaf node (Min_sample_leaf) for XGBoost, were optimized using a grid search algorithm. This algorithm exhaustively searches through a specified subset of the hyperparameter space. We set up a grid of possible values for each hyperparameter to be tuned, as illustrated in the “Specific Search Range” column in Table 2. For each combination of hyperparameters in the grid, the algorithm trains the model using the training data and evaluates its performance through cross-validation. The performance of each hyperparameter combination is measured using several specified evaluation metrics. Finally, the combination of hyperparameters that results in the best performance on the validation set is selected, as shown in the “Optimum Value” column in Table 2. This optimal set of parameters is then used to train the final model on the entire training dataset. For a comprehensive overview of the optimized parameters, refer to Table 2.

<table>
<thead>
<tr>
<th>Table 2. The control parameter for tuning the ML models.</th>
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<tr>
<td>Model</td>
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<td>-------</td>
</tr>
<tr>
<td>RF</td>
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<td></td>
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<td></td>
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<tr>
<td></td>
</tr>
<tr>
<td>XGBoost</td>
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3.3 Model Training and Evaluation

Data partitioning is a pivotal aspect of training and comprehensively assessing the performance of ML algorithms. Two widely adopted techniques for this purpose are Hold-Out and Cross-validation. Hold-Out involves dividing the dataset into training and testing sets using an 80-20 split, ensuring independent model evaluation. On the other hand, Cross-validation, often referred to as 'k-fold,' randomly partitions the data into 'k' groups, thereby enhancing generalization (Yadav and Shukla, 2016).

In this study, we employed a combination of both techniques to evaluate the reliability and stability of the models across spatial and temporal domains. Initially, the dataset underwent division using Hold-Out into an 80% training set and a 20% testing set. Subsequently, a 10-fold cross-validation was conducted on the 80% training data, with eight groups randomly chosen for training and two for model validation.

During the training phase of our ML models, we leveraged datasets spanning diverse temporal periods and geographical regions where both SEVIRI and CALIOP data were accessible. However, following this training phase, the algorithms function autonomously, relying solely on SEVIRI data as their input. This advancement enables us to estimate AOD values at four specified vertical layers within each pixel of the SEVIRI dataset, based on a single SEVIRI observation along with its associated meteorological data and land cover data, covering the entire study area.

Evaluation of the AOD Profiling models involved statistical metrics such as the coefficient of determination ($R^2$), Pearson correlation coefficient (R), root mean square error (RMSE), and mean absolute error (MAE). The selection of the optimal model was based on higher $R^2$ and R values, along with lower RMSE and MAE scores. Additionally, we conducted a validation analysis of AOD Profiling with EARLINET AOD profiles on a continental scale to ascertain the model's performance.

4 Results and Discussion

In this paper, our primary aim is to develop a ML model capable of retrieving AOD across four distinct vertical layers: 1.5, 3, 5, and 10 km. To accomplish this, we utilized two well-established ML models, XGB and RF, previously employed in related studies. These models were trained on SEVIRI data spanning the European continent from 2017 to 2019. Our objective was to estimate sub-hourly AOD values, approximately every 15 minutes, at a spatial resolution of 3 km $\times$ 3 km.

To explore the relationship between AOD and potential predictor variables, we conducted a correlation analysis experiment utilizing the Pearson Correlation Coefficient (PCC, Benesty et al., 2009). Furthermore, we evaluated the influence of land cover and meteorological data as input variables for the ML models in estimating AOD profiles from SEVIRI data, with a specific focus on identifying the most optimal model. Moreover, we conducted training and testing of the ML models across various temporal scales, including annual and seasonal analyses. Subsequently, we assessed the performance of each model using independent satellite and ground-based AOD profiles, employing evaluation metrics such as $R^2$, R, MAE, and RMSE. In the subsequent sections, we will provide a comprehensive review of the results derived from the aforementioned assessments.
4.1 Validation of Estimated AOD with Satellite Retrieval AOD

4.1.1 Feature Importance

According to established radiative transfer theory (Tsang et al., 1984; Zege et al., 1991), the spectral signal captured by a satellite sensor at the top of the atmosphere (TOA) is intricately shaped by various factors, including the composition, size distribution, and altitude of aerosols, as well as atmospheric molecules such as water vapor (WV). These factors directly influence the estimation of AOD values. Hence, SEVIRI reflectance and brightness temperature across bands 1 to 11 were identified as critical features for our analysis. The relationship between AOD and all candidate features was investigated through a correlation analysis experiment, as illustrated in Fig. 5, employing the PCC as the selected filter. The findings underscored that the majority of selected features in this study exhibited significance levels exceeding 1%.

Spatial features, Latitude and Longitude, alongside day, consistently demonstrate high importance to estimate the AOD values across all vertical layers. Lon is the most significant feature in all four cases, with importance ranging from approximately 19.42% to 23.92%. Lat also shows substantial importance, with values between 17.32% and 22.92%. For all four heights, the top three features remain consistent, albeit in different orders: lon, lat, and day. Although the relative importance of these features slightly decreases with height, they remain dominant. Month, year, and various spectral bands (B₁ to B₁₁) also contribute, ranging from 1.63% to 3.86%, to the model. This alignment with previous studies (Kaufman et al., 1997; Hyer et al., 2011; Chen et al., 2022) underscores the robustness of our findings. The importance of these secondary features varies slightly with the height of the AOD layer. For instance, the importance of the month feature is highest at 10 km (5.25%) and lowest at 1.5 km (3.73%). Additionally, meteorological data such as Pressure (P), Temperature (T), Wind Speed (Ws), and Wind Direction (Wd) have relatively low importance across all heights, with contributions below 2% in most cases. Land Cover (LC) is consistently the least important feature in all scenarios. Given the relative importance of meteorological data (P, T, Wd, and Ws) and LC, along with the significant influence of SEVIRI TOA measurements (B₁ to B₁₁), these were retained as input features for our AOD profile retrieval model based on machine learning techniques.
Figure 5. The Importance of input features in the retrieval of SEVIRI AOD profiles, as determined by the Pearson Correlation Coefficient (PCC).

4.1.2 Impact of Meteorological data and Land cover

As previously noted, LC, T, P, Ws, and Wd are key features in AOD estimation. To further understand their impact on ML model performance in SEVIRI AOD profiling, we conducted 16 cases of experiments with varied feature combinations, validated using CALIOP AOD retrievals. Our analysis, depicted in Fig. 6 and supplementary Tables S1-S2, is summarized using statistical metrics like R², R, RMSE, and MAE.

Our findings indicate that, for most cases across annual and seasonal datasets, adding features beyond $B_i$ has negligible impact on the 1.5 km layer. However, integrating T and P features, as seen in cases 3, 4, and 9, notably enhances AOD accuracy at 3, 5, and 10 km altitudes. This improvement is attributed to P reflecting changes in aerosol vertical layers, influencing aerosol diffusion capacity, while T is closely linked to atmospheric aerosol distribution by altering air movement dynamics.

Additionally, our results highlight the superior performance of Case 5, employing Ws and Wd as input wind dynamics features. Incorporating these features significantly enhances R² values across models, with substantial increases ranging from 14 to 89 and 5 to 99 observed in R², and decreases ranging from 3.1 to 1 and 3.5 to 0.2 in RMSE for both XGB and RF models from Case 1 to Case 5 in the 10 km layer. These statistical values underscore the crucial role of wind speed and wind direction in influencing the spatial and temporal properties of atmospheric aerosols, particularly in the 10 km layer.

In comparison to P and T, wind dynamics features exhibit a greater impact on SEVIRI AOD estimation performance, particularly in the 5 and 10 km layers. This is attributed to aerosols' capacity for long-range transport within the atmosphere facilitated by wind-driven advection, particularly in these layers (Nicolae et al., 2019; Georgoulas et al., 2016; Ortiz-Amezcua et al., 2017; Granados-Muñoz et al., 2016). Conversely, LC emerges as an influential confounding feature at 3, 5, and 10 km layers in most models, resulting in a notable reduction in R². This phenomenon arises from the fact that the vertical distribution of aerosols across different atmospheric layers over Europa is more heavily influenced by continental and regional transport patterns, atmospheric stability, and meteorological conditions than localized land cover characteristics (Zhao et al., 2019).

Our model validation using CALIOP AOD retrievals underscores the reliability of our findings, particularly regarding the significance of Ws and Wd in improving AOD estimation accuracy. The consistency of these results across different modeling approaches (RF and XGB, Annual and Seasonal) emphasizes the significance of Ws and Wd in AOD estimation at both 5 km and 10 km layers. Consequently, we prioritize Ws and Wd, along with Bi, as the preferred input features for our models due to their demonstrated impact on improving AOD estimation accuracy.
Figure 6. The impacts of input features on the retrieval of SEVIRI AOD profiles, represented as $R^2$ metrics, for the RF and XGB models. Each row displays the results for the annual period and the four seasons (Winter, Spring, Summer, and Autumn). The four colors in each bar plot indicate the $R^2$ values for AOD at 1.5, 3, 5, and 10 km layers.

4.1.3 Validation of Seasonal Modeling

Given the significant variations in both aerosol distribution and meteorological conditions across seasons, we aimed to investigate whether tailoring our proposed modeling approach to different seasons could enhance the precision of AOD profile retrievals. Following the methodology outlined in Section 3, we partitioned the sample dataset, derived from 2017 to 2019 data, into four segments based on seasonal distinctions: Winter (January, February, and March), Spring (April, May, and June), Summer (July, August, and September), and Autumn (October, November, and December), as detailed in Table 3. Subsequently, we trained individual ML models on these seasonal datasets. Additionally, an annual model was constructed using the entire dataset spanning 2017 to 2019. For this analysis, we separately estimated SEVIRI AOD profiles for the year 2020 using both the seasonal and annual models. The accuracy of these estimations was then assessed using CALIOP AOD retrievals. Detailed seasonal validation findings, including $R^2$ and RMSE metrics, are delineated in Table 4, complemented by supplementary insights and further details on R and MAE available in Table S3.

Table 3. Number of Samples Used to ML models training in this Study.

<table>
<thead>
<tr>
<th>Period</th>
<th>All</th>
<th>Winter</th>
<th>Spring</th>
<th>Summer</th>
<th>Autumn</th>
</tr>
</thead>
<tbody>
<tr>
<td>2017-2019</td>
<td>343489</td>
<td>82752</td>
<td>87358</td>
<td>99750</td>
<td>73629</td>
</tr>
</tbody>
</table>

The XGB model exhibited acceptable performance across different seasons, with $R^2$ (RMSE) values for the 1.5 km layer as follows: 0.930 (0.040 mg/m³) for spring, 0.918 (0.036 mg/m³) for summer, 0.918 (0.046 mg/m³) for autumn, and 0.932 (0.046 mg/m³) for winter. Notably, the RF model showed improvement, boasting $R^2$ values of 0.987, 0.992, 0.994, and 0.994, and corresponding RMSE values of 0.017, 0.011, 0.012, and 0.013 mg/m³ for spring, summer, autumn, and winter, respectively. Similarly, both the XGB and RF models demonstrated satisfactory performance across other layers, with $R^2$ ranging from 0.84 to 0.99, 0.82 to 0.98, and 0.78 to 0.98 for the 3 km, 5 km, and 10 km layers, respectively. Clearly, the performances of models tend to decrease in the upper layers compared to the 1.5 km layer. Due to the prevalent types and sizes of existing aerosols throughout most of the year, with aerosol distribution in Europe predominantly concentrated within the 1.5 and 3 km atmospheric layers. Consequently, $R^2$ and R metrics demonstrate higher values in these layers compared to the 5 and 10 km layers. Conversely, RMSE and MAE metrics are elevated at the 1.5 and 3 km layers but lower at the 5 and 10 km layers. This pattern arises from the typically higher aerosol concentrations occurring in the lower atmospheric layers, juxtaposed with lower AOD values observed in the 5 and 10 km layers.

Table 4. Seasonal performance of proposed AOD profiling ML models.

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However, the XGB Annually model exhibited the RMSE values (0.042 mg/m³, 0.021 mg/m³, 0.015 mg/m³, and 0.015 mg/m³) and the R² values (0.928, 0.908, 0.905, and 0.818). Similarly, the RF Annually model demonstrated significant results, achieving R² values of 0.991, 0.971, 0.983, and 0.996, along with RMSE values of 0.015 mg/m³, 0.012 mg/m³, 0.006 mg/m³, and 0.002 mg/m³, respectively. In conclusion, the effectiveness of AOD profiling models exhibits slight variations in accuracy across seasons compared to annual models. Therefore, we considered the annual models as the desired models to estimate AOD profiles of SEVIRI.

### 4.1.4 Comparison of the models

Figure 7 presents scatterplots illustrating AOD profiles estimated using the proposed annual RF (Fig. 7a-d) and XGB (Fig. 7e-h) models at a wavelength of 530 nm, compared with CALIOP-retrieved AOD profiles over Europe in 2020. Each subplot includes the number of points and mentioned metrics i.e. R², R, RMSE, MAE, Bias, and linear regression equations to facilitate clear and thorough analysis.

Both models exhibit a strong correlation between the estimated values and retrievals. However, the RF model demonstrates slightly superior performance, with R² (R) values of 0.991, 0.971, 0.981, and 0.996 (0.995, 0.986, 0.991, and 0.998) for the 1.5, 3, 5, and 10 km layers, respectively. In comparison, the XGB model shows lower R² (R) values of 0.928, 0.908, 0.905,
and 0.818 (0.994, 0.988, 0.982, and 0.951) for the same layers. While this model demonstrates superior accuracy in estimating AOD within the 1.5 km layer compared to the other layers (3 km, 5 km, and 10 km), the RF model exhibits even greater proficiency in the upper layers, showcasing a notable discrepancy in performance when contrasted with XGB. Notably, the disparity in accuracy between the two models is more pronounced in the upper layers (3 km, 5 km, and 10 km) compared to the 1.5 km layer. This suggests that while both models offer reasonably accurate estimations of AOD in the 1.5 km layer, the RF model excels in capturing the nuances of AOD variability in the upper layers.

Overall, the minimal variation in $R^2$, $R$, RMSE, and MAE across the models suggests comparable estimation capabilities. However, a detailed analysis reveals the superior accuracy of the RF model in capturing AOD values, as evidenced by the slope values in Fig. 7e-h. In contrast, the slope values in Fig. 7a-d indicate that the XGB model tends to slightly underestimate higher AOD values. In summary, while both models demonstrate proficiency, the RF model outperforms the XGB model, particularly in its accuracy for higher altitude layers, thereby providing more reliable AOD estimations.
Figure 7. Scatterplots comparing the estimated SEVIRI AOD profiles derived from the proposed ML models with the CALIOP AOD profiles for the year 2020. The red line represents the linear fit between the two datasets.

4.2 Validation of Estimated AOD with Ground LiDAR Retrievals

To further validate our top-performing models, Annual XGB and RF, we conducted an extensive analysis using data from eight EARLINET stations across Europe in 2020. We focused on pixels within a 3 km radius around each station, centering our comparison and validation on the 550 nm estimated SEVIRI AOD profiles. Figure 8 visually presents the comparison between the estimated SEVIRI and retrieved EARLINET AOD profiles, utilizing a linear regression and metrics including $R^2$, $R$, RMSE, MAE, and Bias. The figure includes four scatterplots of AOD results at 1.5 km, 3 km, 5 km, and 10 km for each model. The XGB model shows better agreement with EARLINET AOD profiles, with $R^2$ values of 0.81, 0.77, 0.71, and 0.56, and RMSE values of 0.03, 0.01, 0.02, and 0.005, respectively. Conversely, the RF model exhibits lower correlation, with $R^2$ values of 0.78, 0.12, 0.43, and 0.07, and RMSE values of 0.028, 0.024, 0.022, and 0.008.

The models were trained using CALIOP data, making them expected to perform effectively when validated with data from the same source. However, significant differences between RF and XGB in feature importance ranking and extraction results (Strobl et al., 2007; Zamani Joharestani et al., 2019) suggest that the RF model may have captured specific characteristics of the CALIOP dataset, contributing to its superior performance in this context. This implies that the RF model might be biased towards the specific patterns and noise characteristics present in the CALIOP training data, leading to decreased performance when applied to the EARLINET data. In contrast, the XGB model appears to generalize to the distinct characteristics of the EARLINET data. This can be attributed to XGB's ensemble nature and its ability to reduce bias through boosting, enabling it to handle complex and diverse datasets more effectively (Ahmed et al., 2023). This adaptability allows the XGB model to perform more accurately with the EARLINET data, resulting in higher $R^2$ values despite the differences from the training data.

In summary, the study demonstrates the superior performance of the XGB model over the RF model in retrieving AOD profiles from the EARLINET data. When comparing the $R^2$ metrics of XGB AODs across different layers, it was found that XGB AODs exhibited lower $R^2$ values with EARLINET at the 10 km layer but showed significant improvement at the 1.5, 3, and 5 km layers, with $R^2$ values of 0.81, 0.76, and 0.71, respectively. This indicates a stronger correlation between XGB AOD estimations and EARLINET retrievals in these layers compared to the 10 km layer, which had an $R^2$ value of 0.56. This trend is consistent with other evaluation metrics. Closely scrutinizing Fig. 8, it becomes apparent that specific points revealing notable discrepancies between EARLINET and XGB AOD profiles are indicated by red rectangles in the subplots. To determine the root cause of these outliers, the data were color-coded based on AOD values, revealing that the majority of outliers occurred when EARLINET retrieved low AOD values in each layer. At these points, the XGB model tends to overestimate. This tendency contributed to a low $R^2$ value (0.56) in the linear regression for the 10 km layer, as this layer contains small AOD values (0-0.05).
Furthermore, the slope of the regression line for XGB model exceeds 1, indicating a consistent underestimation of EARLINET AOD values at the 1.5km layer. In contrast, the slopes for the other layers fall within the range of 0.8 to 0.9. This observation implies that for every unit increase in estimated values, the EARLINET AOD values increase by less than one unit, suggesting a tendency for the estimated values to overestimate the EARLINET AOD in the remaining layers.
Figure 8. Scatterplots comparing the estimated SEVIRI AOD profiles derived from the proposed ML models with the EARLINET AOD profiles across 8 specified stations in Europe for the year 2020. The red line represents the linear fit.
between the two datasets. Note that the scales of the subplots vary due to the different ranges of AOD values at the various vertical layers (1.5, 3, 5, and 10 km).

The statistical analysis of EARLINET AOD profiles at the eight specified stations, alongside estimated SEVIRI AOD profiles, is comprehensively presented in Table 5. The number of analyzed pairs (N) varies across stations, ranging from 12 at HPB to 387 at ATZ, providing robust validation of SEVIRI AOD profiles with EARLINET AOD profiles. Metrics such as RMSE, MAE, and Bias offer valuable insights into model performance at each station. A detailed analysis of the data reveals that the values of these metrics across the four layers are not consistently identical. Discrepancies between the XGB-estimated and retrieved EARLINET AOD values are evident in different layers for each station, as illustrated in Table 5.

Performance varies significantly across stations and layers, with notable discrepancies observed at ATZ (Greece), particularly at the 1.5 km layer, which exhibits the highest RMSE of $3.1 \times 10^{-2}$ mg/m³. The substantial Bias at this station indicates that the model tends to consistently overestimate the AOD at this altitude. Conversely, performance improves at 3 km and 5 km, with RMSE values of $1.5 \times 10^{-2}$ mg/m³ and $1.8 \times 10^{-2}$ mg/m³, respectively. At this station, the model demonstrates the best performance at the 10 km layer, with an RMSE of $0.6 \times 10^{-2}$ mg/m³, compared to the other layers. These variations are likely due to frequent forest fires in Greece, as most smoke from these fires remains in the lower layers of the atmosphere (Nicolae et al., 2019). In contrast, the XGB model generally performs well at the SAL, HPB, and LLE stations, where both RMSE and Bias are minimal. The RMSE at the 1.5 km layer, ranging from $1.1 \times 10^{-2}$ mg/m³ to $2.2 \times 10^{-2}$ mg/m³ at the IPR, WAW, INO, and THE stations, alongside the low RMSE and Bias values across other layers, demonstrates good overall model performance at these stations. A closer examination reveals that RMSE and Bias metrics are often elevated at the 1.5 km and 3 km layers but lower at the 5 km and 10 km layers. This pattern arises from the typically higher aerosol concentrations in the lower atmospheric layers, compared with lower AOD values retrieved in the 5 km and 10 km layers.

The discrepancies between the estimated and retrieved profiles could stem from the different measurement techniques employed by satellite and ground-based systems. EARLINET utilizes ground-based LiDAR systems to capture backscattered light from aerosols within the atmosphere by looking upward, whereas satellite measurements are performed from above, looking down. In this configuration, the lower atmospheric layers attenuate the LiDAR signal, resulting in reduced power to penetrate the upper layers. This attenuation can complicate the detection of aerosols in the upper layers (Grigas et al., 2015; Nicolae et al., 2019). Furthermore, these limitations may be attributed to the constraints associated with the utilization of CALIOP AODs, particularly their reduced precision in low aerosol concentration scenarios. This reduced precision arises from the low signal-to-noise ratio under clean weather conditions, which is often insufficient to accurately detect weak aerosol layers on the aerosol extinction vertical profile. Because both transmitted and scattered light must traverse this portion of the atmosphere, highly diffuse and/or tenuous scattering aerosol layers below the CALIOP detection threshold are ignored in CALIOP's estimates of column AOD. Consequently, weak aerosol layers that are not detected would not be retrieved, leading to decreased retrieved AODs under clean weather conditions (Liu et al., 2018a, b).
Finally, the efficacy of the XGB model is clearly demonstrated by its ability to reliably estimate SEVIRI AOD profiles compared to EARLINET retrieved AOD profiles across various European regions.

<table>
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<th>Station ID</th>
<th>location</th>
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<th>Layer</th>
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<th>RMSE × 10⁻²</th>
<th>Bias × 10⁻²</th>
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</table>
5 Conclusion

This study develops a model that integrates satellite TOA reflectance data from the SEVIRI satellite, meteorological data, and land cover data to estimate vertical AOD across distinct layers of 1.5, 3, 5, and 10 km. Utilizing CALIOP AOD profiles as reference data, models employing RF and XGB were trained on a dataset spanning 2017 to 2019. Subsequently, SEVIRI AOD profiles for 2020 over Europe were estimated and compared with CALIOP and EARLINET AOD products, leading following insight.

Both RF and XGB models demonstrate commendable accuracy in sub-hourly (approximately 15-minute intervals) SEVIRI AOD profile estimation when validated using CALIOP AOD data. However, the RF model exhibits slightly superior performance, with $R^2$ values ranging from 0.971 to 0.995 across the different layers. In comparison, the XGB model outperforms the RF model when compared to EARLINET retrieval AOD profiles, with $R^2$ values ranging from 0.561 to 0.810 across the layers. Additionally, the inclusion of meteorological data (T, P, Ws, and Wd) alongside LC data during model training enhances the performance of the proposed frameworks. These features, often overlooked in physical AOD retrieval methods relying solely on atmospheric radiation transfer models, significantly contribute to refining SEVIRI AOD profile estimates. Notably, wind speed and direction emerge as the most influential meteorological data, leading to increased $R^2$ values and reduced RMSE across all estimated SEVIRI AOD profiles.

In conclusion the XGB model can estimate detailed sub-hourly 3x3 km² SEVIRI AOD profiles, providing valuable insights into aerosol properties. Although our study focuses on Europe and validates the model using ground-based LiDAR data, future research should broaden its application to establish a more generalized approach for AOD retrieval, considering the utilization of an ensemble of geostationary meteorological satellites simultaneously. Additionally, our current model utilized a restricted set of features, overlooking significant factors that influence AOD values, such as precipitation, NDVI, and land use. Enhancing the model’s performance by integrating these additional features is a primary focus of future research.

Data and Material Availability. Data will be made available upon request.

Code availability. Code will be made available on request.

Author Contributions. MP conducted the investigation, design, data curation, and processing, as well as the programming and evaluation. MP also wrote the original draft. MS was responsible for conceptualization, methodology, supervision, and...
validation, and contributed to the review and editing of the manuscript. MMSh contributed to the conceptualization, supervision, and validation of the work. All authors have read and approved the published version of the manuscript.

Competing interests. The authors declare that they have no conflict of interest.

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