

Article

Machine Learning-Based Atmospheric Radiation Calculation Incorporating Earth Curvature

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Highlights

What are the main findings?

- The XGBoost-based mapping model enables accurate and computationally efficient conversion of plane-parallel to spherical atmosphere radiances.
- On the independent large-zenith-angle test subsets (solar zenith angle or viewing zenith angle $\geq 75^\circ$), the model achieved *MAPEs* of no more than 6.53%.

What are the implications of the main findings?

- Feature-importance analysis reveals how viewing geometry, atmospheric optical properties, and aerosol or cloud layer height contribute to spherical radiance predictions under different atmospheric conditions.
- It provides an efficient approach for accounting for Earth-curvature effects in atmospheric radiation calculations of satellite remote sensing applications.

Abstract

Plane-parallel atmospheric radiative transfer models neglect the Earth's curvature, resulting in substantial optical path errors at large zenith angles and limiting the accuracy of satellite remote sensing retrievals. Fully spherical Monte Carlo models can accurately represent curvature and multiple-scattering effects, but their high computational cost limits their application in rapid or operational calculations. Pseudo-spherical approximations offer greater computational efficiency but generally retain plane-parallel assumptions for multiple scattering, which may reduce their accuracy in aerosol- and cloud-laden atmospheres. To address these limitations, this study develops a physics-guided, data-driven framework for efficient spherical radiance estimation. Reference spherical radiances were generated using a Monte Carlo radiative transfer model for representative clear-sky, aerosol-laden, and cloudy atmospheric scenarios. An extreme gradient boosting (XGBoost) model was then trained to map plane-parallel radiances to their spherical counterparts at wavelengths of 450, 550, and 650 nm. The predictors included wavelength, solar zenith angle (SZA), viewing zenith angle, azimuth angle,

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asymmetry factor, surface albedo, optical depth, single scattering albedo, the central height of a single aerosol or cloud layer and plane-parallel radiance. On the independent test set, the XGBoost model achieved a mean absolute percentage error (MAPE) of 5.71%. For the common clear-sky subset used to compare all three methods, the corresponding MAPEs of the plane-parallel and pseudo-spherical models were 29.61% and 19.65%, respectively. These results indicate that the proposed model can substantially reduce curvature-related radiance errors while retaining high computational efficiency across the atmospheric scenarios considered in this study.

Keywords: spherical radiative transfer; Monte Carlo; XGBoost; satellite remote sensing

1. Introduction

The atmospheric radiative transfer model serves as the fundamental support for satellite remote sensing inversion, where its calculation precision dominantly governs the quality and practical applicability of remote sensing datasets. Nevertheless, conventional models generally adopt the plane-parallel atmospheric hypothesis and neglect Earth's curvature characteristics. As illustrated in Figure 1, light rays (such as A-B) travel in an approximate straight path within horizontally homogeneous atmospheric layers in the plane-parallel model, and the path length is determined solely by the zenith angle. In this model, when the viewing zenith angle (VZA) is large ($\geq 75^\circ$), the simulation error in the light path increases significantly because the Earth's curvature effect is neglected [1,2]. For example, when the solar zenith angle is 85° , the radiance error caused by the plane-parallel assumption can reach 12% [3], and this error directly affects the remote sensing accuracy of meteorological satellites. However, in a spherical atmospheric model, the atmosphere forms a spherical structure that envelops the Earth. Light rays (such as C-D and E-F) propagate along radial or nonradial paths on a spherical surface. Owing to the influence of the spherical curvature, the length and direction of their propagation paths differ from those of the straight-line propagation method of the plane-parallel model. Furthermore, during the dawn and dusk periods and in certain high-latitude regions, the large solar zenith angle (SZA) causes the light propagation path to lengthen, and the influence of the spherical atmospheric curvature becomes more pronounced (the path length error in the E-F segment is greater than that in the C-D segment). As shown in Figure 2, the relative differences in radiance between the plane-parallel and spherical atmospheres ($\frac{I^{SS} - I^{PP}}{I^{SS}} \times 100\%$) are significant under high SZA and VZA conditions.

The development of spherical atmospheric models is rooted in the need to eliminate systematic errors inherent in traditional plane-parallel approximations, a challenge that has driven decades of scientific progress. The theoretical foundations for light scattering in a spherical atmosphere were established early by pioneers such as Bellman et al. [4] and Smokty [5]. Shortly after, Rozenberg [6] detailed the spatial ray-tracing required for spherical geometries. However, these foundational mathematical frameworks shared a significant limitation: they largely bypassed the complex dynamics of repeated, multiple scattering events. A crucial paradigm shift occurred when Marchuk adapted the Monte Carlo (MC) technique for atmospheric optics [7]. The MC method solves the radiative transfer problem by stochastically tracing photon histories, including free-path propagation, absorption, scattering by gases, aerosols, and cloud particles, and interactions with atmospheric and surface boundaries. Interaction probabilities are determined by the prescribed optical properties, while scattering directions are sampled from the corresponding phase functions, enabling an explicit representation of complex multiple-scattering processes. In spherical-atmosphere calculations, Earth's curvature is

incorporated directly through the geometry of concentric atmospheric layers and the intersections of photon trajectories with layer interfaces, rather than through an empirical curvature correction [8]. Free from restrictive geometric assumptions, it seamlessly accommodates three-dimensional structures and inhomogeneous profiles. Consequently, MC codes, exemplified by modern tools like MYSTIC, are universally recognized as the reference standards for model validation [9]. Nevertheless, achieving statistical convergence demands the tracking of massive photon ensembles, rendering the MC method computationally prohibitive for rapid, operational data processing [10]. To mitigate these severe processing delays, the scientific community devised a pragmatic hybrid strategy known as the pseudo-spherical approximation (PSS) [11]. It does not solve the radiative transfer equation in a truly spherical atmosphere. Instead, it aims to leverage the computational efficiency of the plane-parallel model, retains the plane-parallel geometric structure for multiple scattering calculations, and delivers results with sufficient accuracy through angular correction. This core concept was prominently implemented in discrete-ordinate solvers like the SCIATRAN model [12]. In this model, PSS functions as a structural bridge between the high accuracy of spherical representations and the computational efficiency of plane-parallel approximations. The SCIATRAN model precisely calculates the primary attenuation of the incoming solar beam using true spherical geometry, but strategically reverts to the computationally cheaper plane-parallel mathematics to evaluate the broader multiple-scattering field. While SCIATRAN drastically cut computation times compared to statistical methods, its reliance on a plane-parallel assumption for secondary scattering means its output reliability degrades sharply when evaluating zenith angles beyond 84° . Pushing the methodology further, Spurr et al. [13,14] integrated spherical corrections into the LIDORT and VLIDORT frameworks, a critical advancement that enabled the rapid simulation of both scalar intensity and polarized vector fields. Despite their widespread utility in remote sensing, independent algorithmic evaluations revealed that these specific pseudo-spherical solvers encounter strict mathematical boundaries, limiting their operational validity to viewing zenith angles below 79.9° [1,2]. Recognizing the persistent inaccuracies at large zenith angles, a modern evolution termed the Improved Pseudo-Spherical Scheme (IPSS) has recently emerged [15]. The IPSS methodology is founded on a core assumption: the ratio of the multiple-scattering component to the single-scattering component remains identical in both plane-parallel and spherical geometries. Exploiting this proportional consistency, the approach first calculates a highly accurate single-scattering solution within a spherical context. It then derives the multiple-to-single scattering ratio under plane-parallel geometry, which is ultimately used to scale the spherical single-scattering field and obtain the total radiation. On this basis, the atmospheric radiation values considering multiple scattering under spherical atmospheric conditions can be derived. While this innovative technique has demonstrated exceptional precision in idealized, pure Rayleigh scattering tests—effectively expanding the envelope for high-angle simulations—its viability remains an open question. Its performance has yet to be rigorously validated in realistic, turbid meteorological conditions dominated by complex aerosol layers and cloud formations, highlighting a critical pathway for future algorithmic refinement.

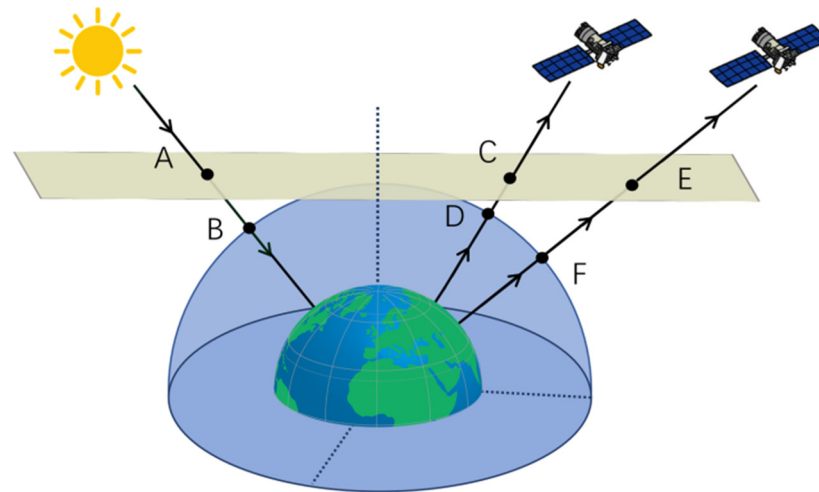


Figure 1. Schematic comparison between spherical and plane-parallel atmospheric models under conditions of high solar zenith angle (SZA) and viewing zenith angle (VZA).

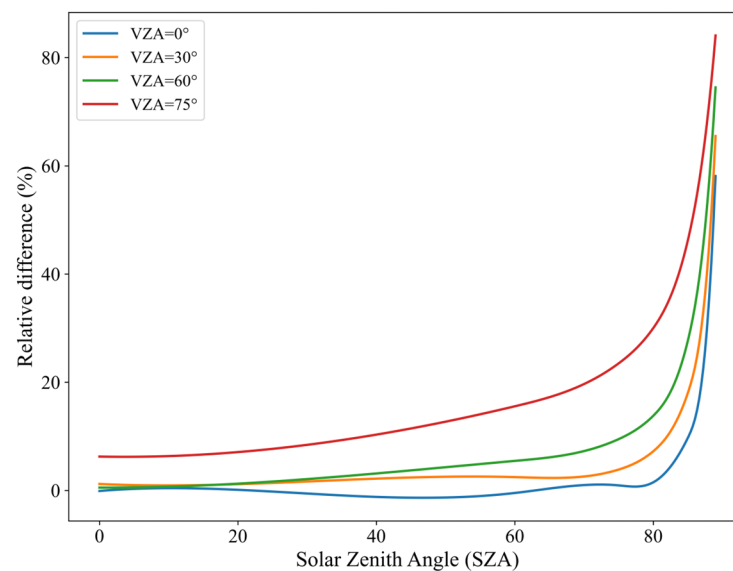


Figure 2. Relative difference (%) in the 450 nm radiance between the plane-parallel (I^{PP}) and spherical (I^{SS}) atmospheric models, assuming a Mid-latitude Summer profile under clear-sky conditions with an azimuth angle of 0° and surface albedo of 0.2.

Recently, with the development of machine learning and the application of atmosphere-related models, combining physical mechanism models and data-driven methods has ingeniously solved several problems. For example, Lagerquist et al. developed knowledge-guided U-net++ deep learning models to emulate the shortwave Rapid Radiative Transfer Model (RRTM). This physics-informed approach successfully predicted radiative fluxes and heating rates for numerical weather prediction while accelerating the computation by approximately four orders of magnitude (10^4 times) compared to the original physical solver [16]. Similarly, to address the immense computational burden of complex three-dimensional (3D) cloud geometry, Weber et al. combined a novel spatial approximation (IDEFAX) with artificial neural networks to create a fast forward operator for polarized 3D radiative transfer. This method significantly improved the representation of 3D cloud radiative effects while operating about five orders of magnitude (10^5 times) faster than rigorous 3D simulations [17]. Furthermore, Pal et al. implemented deep neural networks as cost-effective surrogate models for both shortwave and longwave radiative transfer in the Super-Parameterized

Energy Exascale Earth System Model (SP-E3SM), which reproduced radiation parameters with 90–95% accuracy at an 8–10 times reduced computational cost [18]. Therefore, this study focuses on the nonlinear characteristics of the spherical atmospheric radiative transfer equation, accounting for the influence of physical parameters such as wavelength (λ), solar zenith angle (SZA), viewing zenith angle (VZA), azimuth angle (PHI), asymmetry factor (g), surface albedo (α_s), optical depth (τ), single scattering albedo (SSA), central height (h) on the intensity. A Monte Carlo model is employed to generate high-precision labeled data, which in turn is used to train a machine learning model designed to replace traditional numerical iterative calculations. The core mechanism of the Monte Carlo spherical model involves producing high-precision radiation field annotation data through random photon tracking and spherical curvature correction. This data-driven approach effectively substitutes iterative numerical calculations based on plane-parallel or pseudo-spherical approximations, thereby addressing the problem of cumulative systematic errors introduced by geometric simplification at large zenith angles.

2. Dataset and Methods

2.1. Dataset

2.1.1. Input Parameters

The core elements of the dataset include the input parameters and output radiance. The input parameters include λ , SZA, VZA, PHI, g , τ , SSA, α_s , h and I^{PP} [19]. The target output is the intensity of spherical radiance under the corresponding parameter combinations.

The selection of λ was based on the key visible light channel center wavelengths of the Medium Resolution Spectral Imager-III (MERSI-III) onboard the Fengyun-3F (FY-3F) satellite (National Satellite Meteorological Centre, Beijing, China). Wavelengths of 450, 550, and 650 nm were selected because they are highly sensitive to the scattering characteristics of atmospheric aerosols and cloud particles. The SZA ranged from 0° to 89°, with enhanced sampling density in the high SZA range from 70° to 89° (see Table 1) to examine the significant differences between spherical and plane-parallel atmospheres at low solar altitude, such as sunrise or sunset. The VZA varied between 0° and 79°, with enhanced coverage of large VZAs (>60°) near the horizon to capture radiance changes caused by differences in the geometric path curvature.

For clear-sky simulations, the atmosphere was modeled assuming the dominance of molecular (Rayleigh) scattering. The optical depth was characterized based on gas abundance information from 0 to 120 km across six standard atmospheric profiles: mid-latitude summer, mid-latitude winter, sub-arctic summer, sub-arctic winter, tropical, and U.S. Standard. Specifically, for a clean and clear atmosphere, the influence of optical depth is quantified by integrating the content of key gases over their primary influencing altitudes: total column air, ozone (O₃) concentration in the ozone layer, water vapor (H₂O) concentration below 500 hPa (0–6 km for model data), and total column oxygen (O₂) concentration.

Representative data from common aerosol and cloud types were selected with the aim of investigating the impact of different vertical structures on the radiative effect to enhance model accuracy. Aerosol optical parameters were derived from the Optical Properties of Aerosols and Clouds (OPAC) database (<https://geisa.aeris-data.fr/opac/>, accessed on 2 June 2025). To broaden the range of aerosol optical properties represented in model development, four aerosol components from the OPAC database were considered: soluble sulfate aerosols (SUSO), sea-salt coarse-mode aerosols (SSCM), soot (SOOT), and water-soluble aerosols (WASO) [20]. Our selection criteria were specifically designed to span contrasting optical regimes, covering fine-mode weakly absorbing

particles, strongly absorbing carbonaceous particles, and coarse-mode marine particles. Thus, the selection provides variations in particle size, single-scattering albedo, and scattering asymmetry while maintaining a computationally manageable parameter space. However, this selection was not intended to represent all globally important aerosol categories. Mineral aerosol was not included because its adequate representation would require consideration of multiple size modes, variable mineral compositions, and nonspherical scattering phase functions, which were beyond the scope of the present dataset, as further discussed in Section 5. For each type, the *SSA* and *gg* values were assigned based on the standard optical models defined in the OPAC database. By coupling these intrinsic properties with the variable optical depth (τ), the simulation effectively captures the spectral behavior of different aerosol loadings. The cloudy cases encompassed both cumulus and cirrus types, with microphysical data referred to the OPAC database and some references [21–23]. By configuring cumulus and cirrus clouds at various altitudes, the dataset simulates vertical structural variations in actual cloudy atmospheres.

Due to the significant influence of the vertical distribution of aerosols or clouds on radiative transfer under non-clear-sky atmospheric conditions in spherical geometry, this study introduces a key parameter: the central height (h), with the unit of kilometers (km). It denotes the center altitude of the added aerosol or cloud layer (from the surface), effectively constraining its vertical position within the atmospheric column. Furthermore, regarding the vertical extent, the layer thickness (Δz) is uniformly set to 1 km across all experiments in this study. This means that aerosols or clouds are restricted to a single 1 km layer at a time, precluding simultaneous additions across multiple layers. This single-layer assumption with a fixed thickness is adopted to simplify the theoretical discussion and isolate the explicit impact of the layer's altitude on the radiative transfer process.

Table 1. List of input parameters used in the experiment under different atmospheric conditions. The single scattering albedo (*SSA*) and asymmetry factor (*gg*) for aerosol-laden atmosphere, along with the *SSA* for cloudy atmospheres, are derived from the OPAC database (<https://geisa.aeris-data.fr/opac/>, accessed on 2 June 2025). All remaining physical quantities are prescribed experimental settings in this study.

Input Parameters		Values/Options
Wavelength, Geometric Angle, Surface Information	Wavelength (λ)	450 nm, 550 nm, 650 nm
	Solar Zenith Angle (<i>SZA</i>)	0°, 30°, 60°, 70°, 73°, 75°, 77°, 80°, 82°, 85°, 86°, 87°, 88°, 89°
	Viewing Zenith Angle (<i>VZA</i>)	0°, 30°, 60°, 75°, 79°
	azimuth angle (<i>PHI</i>)	0°, 90°
	Surface Albedo (α_s)	0.08 (ocean), 0.2 (grass), 0.8 (snow) [24]
Clear and Clean Atmosphere	Atmospheric Profiles	Vertical concentration profiles of various atmospheric trace gases are defined and preset based on six atmospheric profiles built into the libRadtran radiative transfer software package, including mid-latitude summer, mid-latitude winter, sub-arctic summer, sub-arctic winter, tropical, and U.S. Standard atmospheres [9].
	Typical Aerosol Types	SUSO (Soluble sulfate aerosols), WASO (water-soluble aerosols), SOOT (black carbon), SSCM (sea salt coarse mode aerosols)
Aerosol-Laden Atmosphere	Optical Depth (τ)	Prescribed according to the microphysical properties from OPAC database [20] (log-normal size distribution and complex refractive indices at RH = 50%), the number concentrations of each aerosol type, as well as λ , Δz and h adopted in the experiment: SUSO: [0.1738, 0.228] WASO: [0.116, 0.197] SOOT: [0.0395, 0.0666] SSCM: [0.0229, 0.0232] (450 nm): 0.99999992 (SUSO), 0.9808 (WASO), 0.2456 (SOOT), 0.99999587 (SSCM)

Cloud Atmosphere	Single Scattering Albedo (SSA)	(550 nm): 0.99999993 (SUSO), 0.9765 (WASO), 0.2088 (SOOT), 0.99999855 (SSCM) (650 nm): 0.99999982 (SUSO), 0.9715 (WASO), 0.1756 (SOOT), 0.99999264 (SSCM)
	Asymmetry Factor (gg)	(450 nm): 0.772 (SUSO), 0.687 (WASO), 0.374 (SOOT), 0.852 (SSCM) (550 nm): 0.769 (SUSO), 0.672 (WASO), 0.336 (SOOT), 0.846 (SSCM) (650 nm): 0.763 (SUSO), 0.656 (WASO), 0.305 (SOOT), 0.845 (SSCM)
	Central Height (h)	SUSO: [0.5, 2.5] WASO: [0.5, 2.5] SOOT: [0.5, 1.5] SSCM: [0.5, 1.5]
	Optical Depth (τ)	Prescribed according to previous studies [21]: Cumulus: 9.4 Cirrus: 2.0
	Single Scattering Albedo (SSA)	SSAs at 450, 550, and 650 nm are set to 0.9999999
	Asymmetry Factor (gg)	Prescribed according to previous studies: Cumulus: 0.855 (450 nm), 0.854 (550 nm), 0.848 (650 nm) [22] Cirrus: 0.796 (450 nm), 0.799 (550 nm), 0.802 (650 nm) [23]
	Central Height (h)	Cumulus: [1.5, 2.5] Cirrus: [6.5, 11.5]

2.1.2. Data Processing

All radiance data were generated using the well-established and widely recognized atmospheric radiative transfer calculation software package libRadtran (version 2.0.4) [9]. This platform integrates multiple rigorously validated algorithms to solve radiative transfer equations. The Monte Carlo radiative transfer algorithm [25], MYSTIC, built into the libRadtran software package, was uniformly used to generate radiance data at the top of the atmosphere for the plane-parallel (I^{PP}) and spherical-atmosphere (I^{SS}) cases. This study adopted six representative standard atmospheric profiles: Tropical, Mid-latitude Summer, Mid-latitude Winter, Sub-arctic Summer, Sub-arctic Winter, and U.S. Standard Atmosphere. The atmospheric column was discretized into 50 vertical layers spanning from the surface up to the top of the atmosphere at 120 km, utilizing a non-uniform vertical grid spacing (with finer resolution in the lower troposphere) to better resolve the high-gradient regions. Spherical atmospheric radiative transfer simulations were conducted using the Monte Carlo approach in backward mode (MYSTIC with the mc_spherical 1D option). Depending on the atmospheric configuration, the number of simulated photons was set to 10,000 for clear and aerosol-laden atmospheres, and 100,000 for cloudy atmospheres. These settings were found to be sufficient to ensure statistical convergence while maintaining computational feasibility for the large number of cases considered. Through systematic parameter configuration and precise calculations using libRadtran, a paired dataset was generated that covered various spectral, geometric (particularly at large angles), and atmospheric optical properties (clean, clouds, and various aerosols) (Table 1). This dataset includes λ , SZA , VZA , PHI , gg , τ , SSA , α_s , h , I^{PP} , and I^{SS} , which comprehensively characterize the differences in radiation response between the plane-parallel and spherical models under various conditions.

To ensure the consistency and reliability of the simulated radiative fields prior to model training, the raw dataset underwent a structured multi-stage cleaning process. First, all numerical variables were screened and any record containing negative values was removed to eliminate physically invalid results. Second, since I^{SS} and I^{PP} describe the same radiative field under different geometric assumptions and should therefore be of comparable magnitude, a physical consistency check was performed by evaluating their ratio:

$$R = \frac{I^{SS}}{I^{PP}}, \quad (1)$$

Records with ratios outside the plausible range (0.05–20), meaning that the difference between I^{PP} and I^{SS} should not exceed a factor of 20, were classified as unreliable. Such deviations typically stem from the intrinsic stochastic noise of the MYSTIC solver—most pronounced under conditions involving highly forward-scattering aerosols, or extreme solar-viewing geometries where limited photon statistics can yield unstable radiance estimates. Additionally, when SSA approaches 1, photons undergo repeated scattering with minimal absorption, greatly increasing scattering events and amplifying Monte Carlo variance, further contributing to numerical instability. Samples affected by these issues were therefore removed to maintain physical coherence in the dataset. Third, to reduce the impact of anomalously large values on model fitting, the upper 0.1% tail of I^{SS} was examined. When the 99.9th percentile exceeded ten times the median, the corresponding records were discarded to prevent extreme radiance spikes from dominating the learning process. Through these steps, after filtering out approximately 1.40% of the data, a physically consistent and statistically robust dataset was obtained for subsequent model development.

2.2. Methods—XGBoost

XGBoost is an ensemble learning algorithm developed for diverse data science and machine learning tasks and performs exceptionally well when handling structured data. The algorithm combines multiple weak learners to create a strong model and iteratively adds decision trees to build a robust predictive model. The core concept of XGBoost is to use a gradient boosting framework to construct a model by progressively reducing its prediction errors. In each iteration, the residuals of the current model were calculated, and a new decision tree was fitted based on the residual results. This process was repeated until the model's performance stabilized or a predefined number of iterations was reached.

Based on the aerosol and cloud configurations described above, the input feature set was defined to represent the atmospheric optical properties and illumination–observation geometries relevant to spherical radiative transfer. The radiance in a spherical atmosphere (I^{SS}) is influenced by a suite of fundamental physical parameters, including λ , SZA , VZA , PHI , gg , τ , SSA , α_s and h . In addition to these variables, the radiance simulated using the plane-parallel approximation (I^{PP}) was included as a physically informed predictor. Although I^{PP} is determined by the aforementioned physical parameters, it provides a baseline radiance that incorporates their combined effects under plane-parallel geometry. The XGBoost model was therefore trained to learn the nonlinear mapping from I^{PP} and the associated physical parameters to the corresponding spherical-atmosphere radiance I^{SS} . Figure 3 shows the analysis and modeling process of XGBoost for addressing atmospheric radiation transport problems, primarily encompassing data preprocessing, dataset partitioning, parameter tuning, model training, and evaluation.

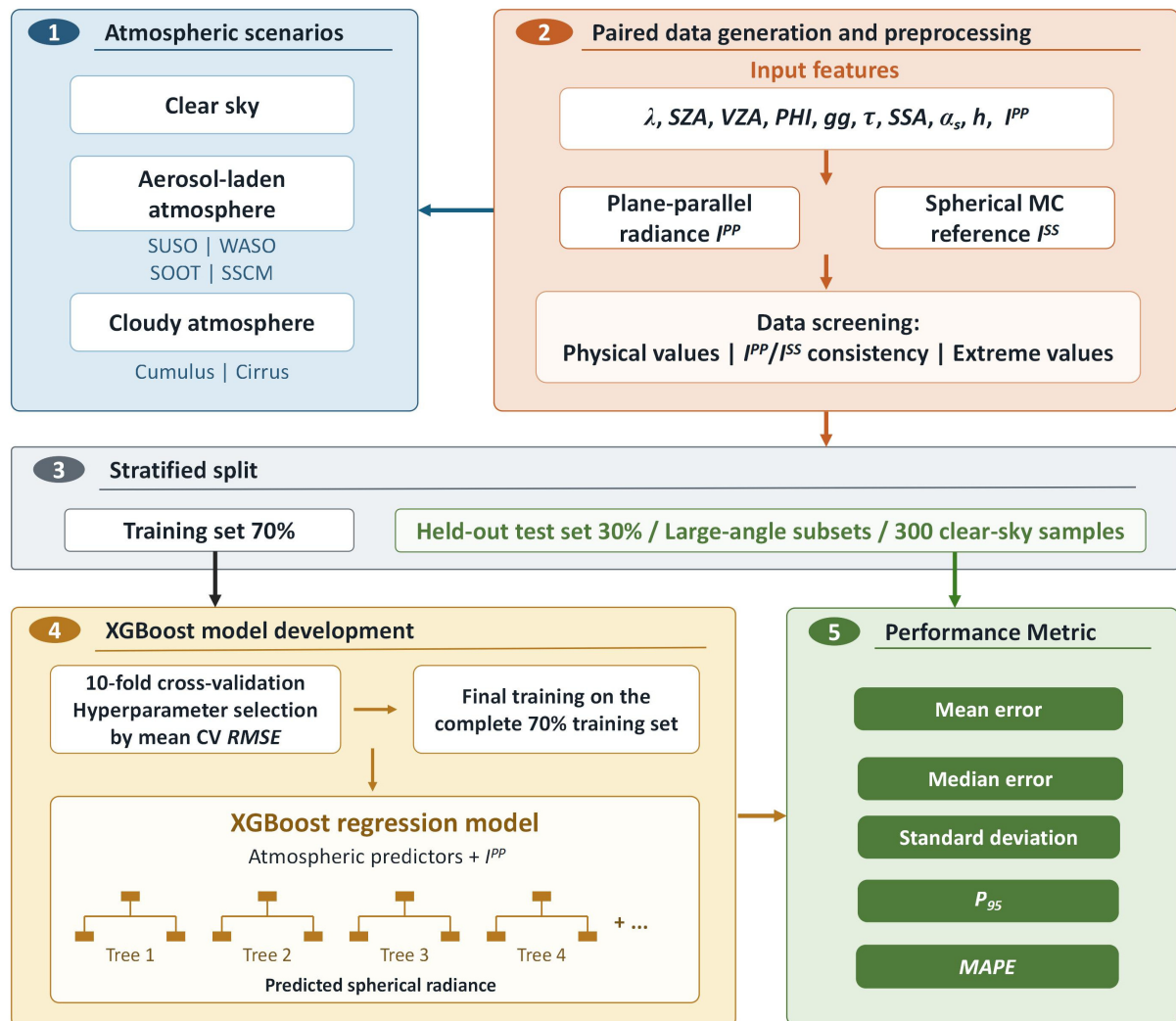


Figure 3. Workflow for dataset construction, XGBoost model development, hyperparameter optimization, and independent test-set evaluation.

2.3. Evaluation Metrics

In regression problems, XGBoost typically uses the root mean square error (RMSE) as the primary loss function, and the RMSE and coefficient of determination (R^2) are commonly used metrics for evaluating regression model performance [26]. The specific formulas are as follows:

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2}, \quad (2)$$

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2}, \quad (3)$$

where n represents the sample size, y_i denotes the actual value of the i -th sample, $\hat{y}_i$ represents the predicted value of the i -th sample, and $\bar{y}$ is the average of the actual values. The RMSE is the square root of the average of the squares of the differences between the predicted and actual values and is used to measure the magnitude of the model's prediction error. The smaller the RMSE, the higher the prediction accuracy of the model. R^2 is a statistical measure of the goodness of fit of the regression model. The closer the value of R^2 is to 1, the better the model fit. Furthermore, to quantitatively compare the simulation performance of different models, multiple statistical metrics are adopted in this study, including the mean error, median error, standard deviation, 95th percentile

relative error (P_{95}), and mean absolute percentage error ($MAPE$). The mean error and median error characterize the average and intermediate levels of the error distribution, respectively, and jointly describe the central tendency of model bias. The standard deviation quantifies the dispersion of model errors; a smaller standard deviation corresponds to a more concentrated error distribution, indicating stable predictive performance under various simulation conditions. P_{95} corresponds to the value below which 95% of the absolute relative errors fall, evaluating the tail of the error distribution rather than the average performance. It reflects the upper bound of the prediction error magnitude for the vast majority of the data, whereby a lower value signifies robust model performance with effectively constrained large-error outliers. Mathematically, the absolute relative error (ARE) for each sample is first calculated as

$$ARE = \left| \frac{\hat{y}_i - y_i}{y_i} \right| \times 100\%, \quad (4)$$

where y_i and $\hat{y}_i$ denotes the true and predicted values, respectively. After sorting the ARE of all N samples in ascending order $ARE_{(1)} \leq ARE_{(2)} \leq \dots \leq ARE_{(N)}$, P_{95} is extracted as

$$P_{95} = ARE_{(k)}, \text{ where } k = \lceil 0.95 \times N \rceil, \quad (5)$$

with $\lceil \cdot \rceil$ representing the ceiling function. $MAPE$ quantifies the average relative deviation between model predictions and reference true values [26], and is defined as

$$MAPE = \frac{1}{n} \sum_{i=1}^n \left| \frac{\hat{y}_i - y_i}{y_i} \right| \times 100\%, \quad (6)$$

where n represents the total number of samples, y_i and $\hat{y}_i$ denotes the true and predicted values, respectively. A smaller $MAPE$ signifies higher overall prediction accuracy.

3. Model Implementation and Training

In the model, based on the physical parameters involved in simulating different atmospheric conditions using libRadtran, the ten attributes: wavelength (λ), solar zenith angle (SZA), viewing zenith angle (VZA), azimuth angle (PHI), asymmetry factor (gg), surface albedo (α_s), optical depth (τ), single scattering albedo (SSA), central height (h), and plane-parallel radiance (I^{PP}) were chosen as the feature variables X . Spherical radiance (I^{SS}) was chosen as the target variable Y . To ensure comprehensive coverage of atmospheric radiative conditions, the dataset (12,517 samples in total) is categorized into three major atmospheric types: clear atmosphere, aerosol-laden atmosphere (SUSO, WASO, SOOT, and SSCM) and cloud atmosphere, which comprises both cumulus and cirrus. The distribution of samples across these categories is shown in Figure 4.

After extracting the relevant variables, the dataset was divided through stratified random sampling into a training set (70%) and an independent test set (30%), while preserving the proportions of clear, aerosol-laden, and cloudy cases. Hyperparameter optimization was conducted exclusively on the training set using 10-fold cross-validation to reduce the sensitivity of model selection to a particular data partition. A hyperparameter grid was constructed for the number of estimators, maximum tree depth, learning rate, subsampling ratio, and column sampling ratio. Candidate configurations were evaluated according to their mean cross-validation $RMSE$, and the effects of different hyperparameter combinations on model performance are visualized in Figure 5. Within the investigated parameter range, the mean cross-validation $RMSE$ generally decreased as the number of estimators increased, reaching its minimum value when 300 estimators were used. The selected hyperparameters are summarized in Table 2. Under this

configuration, the model achieved a mean 10-fold cross-validation $RMSE$ of $4.7524 \pm 4.4057 \text{ W m}^{-2} \text{ sr}^{-1} \text{ nm}^{-1}$ and an R^2 of 0.9987 ± 0.0078 across the validation folds of the training set. Finally, the model was retrained on the entire training set using the selected hyperparameters and evaluated once on the untouched independent test set.

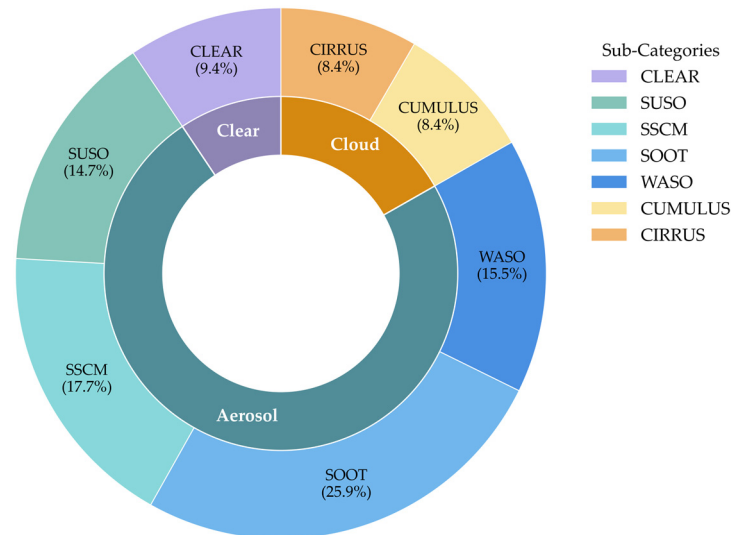


Figure 4. Distribution of three atmospheric conditions in the dataset.

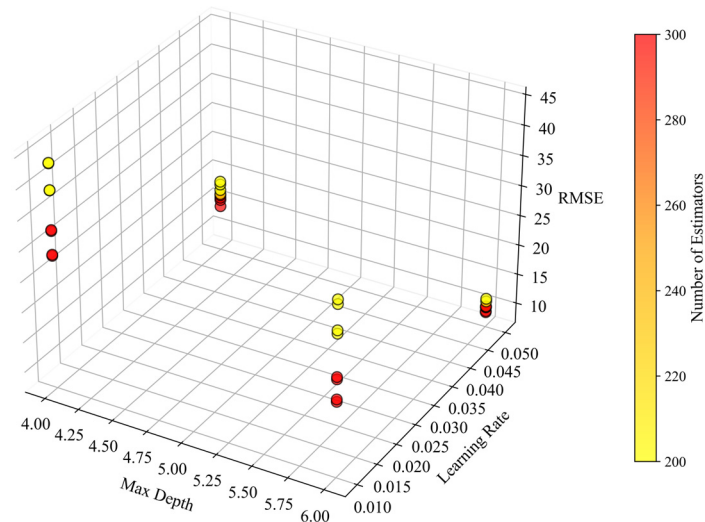


Figure 5. Influence of hyperparameter settings on $RMSE$. The x-axis denotes the maximum depth of decision trees, the y-axis represents the learning rate, the z-axis corresponds to $RMSE$ values, and color intensity indicates the number of estimators.

Table 2. Optimal combination of hyperparameters.

Hyperparameters	Value
Column Sample by Tree	1
Learning Rate	0.05
Maximum Depth	6
Number of Estimators	300
Subsample	0.7

4. Results and Validation

After hyperparameter selection, the final XGBoost model was evaluated on the untouched independent test set, which comprised 30% of the complete dataset and included clear-sky, aerosol-laden, and cloudy cases ($N = 3703$). The spherical radiances calculated using the Monte Carlo model (I^{SS}) were treated as the reference values. For each test sample, the radiance predicted by the XGBoost model and the corresponding plane-parallel radiance (I^{PP}) were compared with I^{SS} . Model performance was evaluated using five metrics: mean error, median error, error standard deviation, the 95th percentile of the absolute relative error (P_{95}), and mean absolute percentage error (MAPE). The results are summarized in Table 3.

Table 3. Performance of the XGBoost-based and plane-parallel radiance estimates relative to the Monte Carlo spherical radiances on the independent test set.

Performance Metric	Plane-Parallel Model	XGBoost-Based Model
Mean Error ($\text{W m}^{-2} \text{sr}^{-1} \text{nm}^{-1}$)	38.96	4.06
Median Error ($\text{W m}^{-2} \text{sr}^{-1} \text{nm}^{-1}$)	7.39	1.72
Standard Deviation ($\text{W m}^{-2} \text{sr}^{-1} \text{nm}^{-1}$)	81.39	8.19
P_{95} (%)	81.63	17.54
MAPE (%)	29.06	5.71

As shown in Table 3, the XGBoost-based model consistently outperformed the plane-parallel approximation on the complete independent test set. The magnitude of the mean error decreased from $38.96 \text{ W m}^{-2} \text{sr}^{-1} \text{nm}^{-1}$ for the plane-parallel model to $4.06 \text{ W m}^{-2} \text{sr}^{-1} \text{nm}^{-1}$ for the XGBoost model, while the error standard deviation decreased from 81.39 to $8.19 \text{ W m}^{-2} \text{sr}^{-1} \text{nm}^{-1}$. The XGBoost model also reduced P_{95} from 81.63% to 17.54% and MAPE from 29.06% to 5.71%. These reductions indicate that the proposed model not only corrected much of the systematic bias associated with the plane-parallel approximation but also reduced the overall dispersion and upper-tail magnitude of the prediction errors across the clear-sky, aerosol-laden, and cloudy cases represented in the test set.

Having established the overall performance of the XGBoost model on the complete independent test set, we further examined its robustness under large-zenith-angle conditions, where the errors associated with the plane-parallel approximation are expected to become more pronounced. Two subsets were extracted from the same independent test set: one containing samples with $SZA \geq 75^\circ$ ($N = 2753$) and the other containing samples with $VZA \geq 75^\circ$ ($N = 1447$). No additional model training or hyperparameter adjustment was performed for these subsets. The XGBoost radiances were evaluated against the corresponding Monte Carlo spherical radiances using the same five performance metrics as those applied to the complete test set. The results are summarized in Table 4.

Table 4. Statistical metrics of the XGBoost model for the large-angle cases with $SZA \geq 75^\circ$ and $VZA \geq 75^\circ$.

Performance Metric	$SZA \geq 75^\circ$	$VZA \geq 75^\circ$
Mean Error ($\text{W m}^{-2} \text{sr}^{-1} \text{nm}^{-1}$)	4.21	7.65
Median Error ($\text{W m}^{-2} \text{sr}^{-1} \text{nm}^{-1}$)	1.61	4.67
Standard Deviation ($\text{W m}^{-2} \text{sr}^{-1} \text{nm}^{-1}$)	9.11	11.87
P_{95} (%)	20.25	14.32
MAPE (%)	6.53	6.03

Compared with its performance on the complete test set, the XGBoost model retained relatively stable accuracy under both large-SZA and large-VZA conditions. The MAPE and P_{95} remain constrained within 6.53% and 20.25%, respectively. This proves that the XGBoost model successfully captures and corrects the complex non-linear spherical geometric effects that typically cause traditional models to fail under large solar and viewing zenith angles.

After evaluating the overall and large-angle performance on the complete independent test set, we further compared it with the pseudo-spherical approximation using a common clear-sky subset. Because the pseudo-spherical approximation retains a plane-parallel treatment of multiple scattering, the three-model comparison was restricted to 300 clear-sky samples to avoid conflating curvature-related effects with the stronger multiple-scattering effects of aerosols and clouds. Pseudo-spherical radiances for these samples were calculated using the pseudo-spherical DISORT solver with 16 streams. The plane-parallel, pseudo-spherical, and XGBoost results were evaluated against the same Monte Carlo spherical radiances, as shown in Figures 6 and 7.

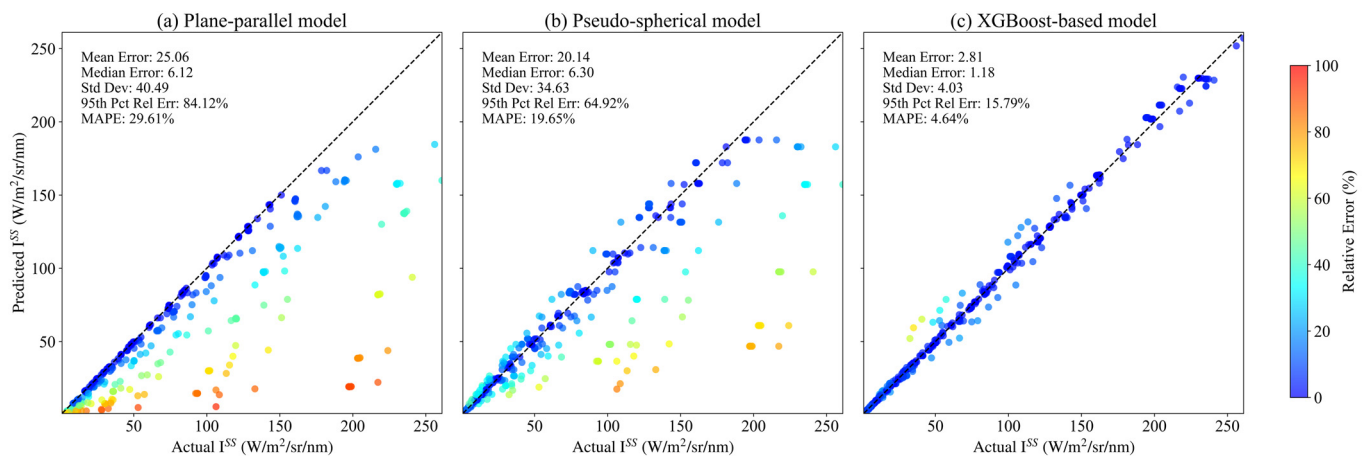


Figure 6. Scatter plots of (a) Plane-parallel radiance (I^{PP}) and Monte Carlo reference radiance (I^{SS}); (b) Pseudo-spherical radiance (I^{PS}) and Monte Carlo reference radiance (I^{SS}); (c) Machine learning predicted radiance and Monte Carlo reference radiance (I^{SS}). The black dotted line represents the reference line for perfect agreement, and the shade of the scatter plot colors indicates the absolute relative error (%). Comparisons are from 300 clear-sky samples.

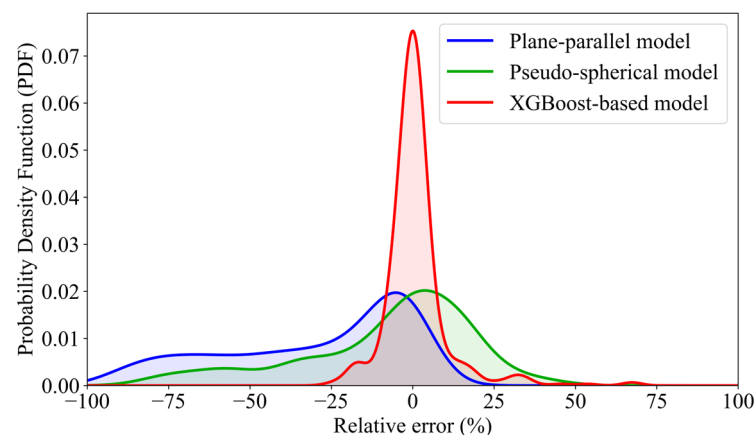


Figure 7. Probability density distributions of the relative errors for the three predictive models. The curves represent the error distributions for the plane-parallel model (blue), pseudo-spherical model (green), and XGBoost-based model (red).

A comparison of the three models shows that the conventional plane-parallel model (Figure 6a) and pseudo-spherical model (Figure 6b) exhibit substantial deviations from the 1:1 reference line, particularly showing a tendency to underestimate radiance at higher actual values. This is quantitatively indicated by their relatively high *MAPE* (29.61% and 19.65%, respectively) and 95th percentile relative errors (84.12% and 64.92%, respectively). In contrast, the XGBoost-based model (Figure 6c) achieves a much closer alignment with the Monte Carlo reference radiance. Its scatter points are tightly distributed along the diagonal reference line, with the predominant blue coloration indicating low relative errors across the entire radiance range. With a mean error of $2.81 \text{ W m}^{-2} \text{ sr}^{-1} \text{ nm}^{-1}$, a *MAPE* of 4.64%, and 95% of its predictions falling within a 15.79% relative error, the machine learning model demonstrates a strong capability to capture the complex mapping between the input variables and the target outputs for the 300 samples, offering a more consistent and reliable alternative to traditional physical approximation models.

To identify the angular conditions under which conventional radiative transfer approximations produce relatively large errors and to quantify the corresponding improvement achieved by the machine-learning approach, Table 5 stratifies the *MAPE* across low, moderate, and large angle ranges for *SAZ*. The *MAPE* values of both the plane-parallel and pseudo-spherical models increase with *SAZ*, with their largest relative errors occurring in the large-angle regime. In this range, the *MAPE* of the plane-parallel model reaches 38.67%. Although the pseudo-spherical model mitigates this to some extent, it still yields considerable errors of 24.35%. This increase is consistent with the growing importance of curved atmospheric paths under oblique solar illumination. The plane-parallel model neglects Earth curvature, whereas the pseudo-spherical approximation does not fully represent spherical geometry for all scattering paths. In contrast, the XGBoost-based model yields a *MAPE* of 5.78% in the large-angle range. Relative to the plane-parallel model, this represents an absolute reduction of 32.89 percentage points, corresponding to an 85.05% relative reduction in *MAPE*. Compared with the pseudo-spherical model, the corresponding reductions are 18.57 percentage points and 76.26%, respectively. These results indicate that, within the atmospheric and angular ranges represented in the dataset, the improvement provided by XGBoost is greatest at large *SAZ*, whereas the improvement is comparatively smaller at low *SAZ*.

Table 5. Comparison of *MAPE* (%) for the three models across different *SAZ* ranges. Comparisons are from 300 clear-sky samples.

Models	Low-Angle Range	Moderate-Angle Range	Large-Angle Range
	<i>SAZ</i> ∈ [0°, 60°)	<i>SAZ</i> ∈ [60°, 75°)	<i>SAZ</i> ∈ [75°, 89°]
Plane-Parallel Model	4.87	10.10	38.67
Pseudo-spherical Model	6.16	10.21	24.35
XGBoost-based Model	2.64	2.48	5.78

For the common subset of 300 clear-sky test samples, Figure 7 compares the probability density distributions of relative errors by the three models. The plane-parallel error distribution is broad and concentrated predominantly on the negative side of zero, indicating a systematic tendency to underestimate the Monte Carlo spherical radiances. The pseudo-spherical distribution is shifted closer to zero but remains relatively broad, suggesting that the spherical treatment of the direct solar beam reduces, but does not eliminate, the radiance errors. In contrast, the error distribution of the XGBoost model is substantially narrower and more closely centered on zero, indicating smaller systematic bias and lower error dispersion.

To examine the relative contributions of different predictors, Figure 8 categorizes and ranks the feature importance affecting spherical atmospheric radiance predictions under

clear and non-clear atmospheric scenarios. In Figure 8a for clear atmospheric conditions, I^{PP} exhibited the highest importance at 26.6%, indicating that it provided the primary predictive baseline for estimating spherical radiance. λ (19.6%) followed closely, reflecting the strong wavelength dependence of Rayleigh scattering by atmospheric molecules. The substantial importance of VZA (17.4%) and SZA (14.4%) is consistent with the sensitivity of radiance to illumination–viewing geometry and atmospheric path length, followed by α_s (13.4%) and Φ (8.6%). This illustrates that the discrepancy between spherical and plane-parallel radiative transfer in clear skies is fundamentally a geometric path-length effect governed by viewing geometries and Earth’s curvature. Under non-clear atmospheric conditions shown in Figure 8b, while I^{PP} maintained its baseline importance (26.6%), the ranking of physical parameters shifted significantly. τ (18.2%) emerged as the second most critical feature, and h (12.0%) also made a substantial contribution to the model prediction. This shift indicates that the model relies more strongly on the optical loading and vertical location of aerosol and cloud layers under non-clear atmospheric conditions. This behavior is consistent with the expected effects of optical depth and layer height on multiple scattering and photon propagation paths. Notably, the importance of λ and α_s dropped drastically to only 1.5% and 1.0%, respectively. These lower scores indicate that λ and α_s provided smaller incremental contributions after the other predictors were considered; they do not imply that wavelength dependence or surface reflection is physically negligible.

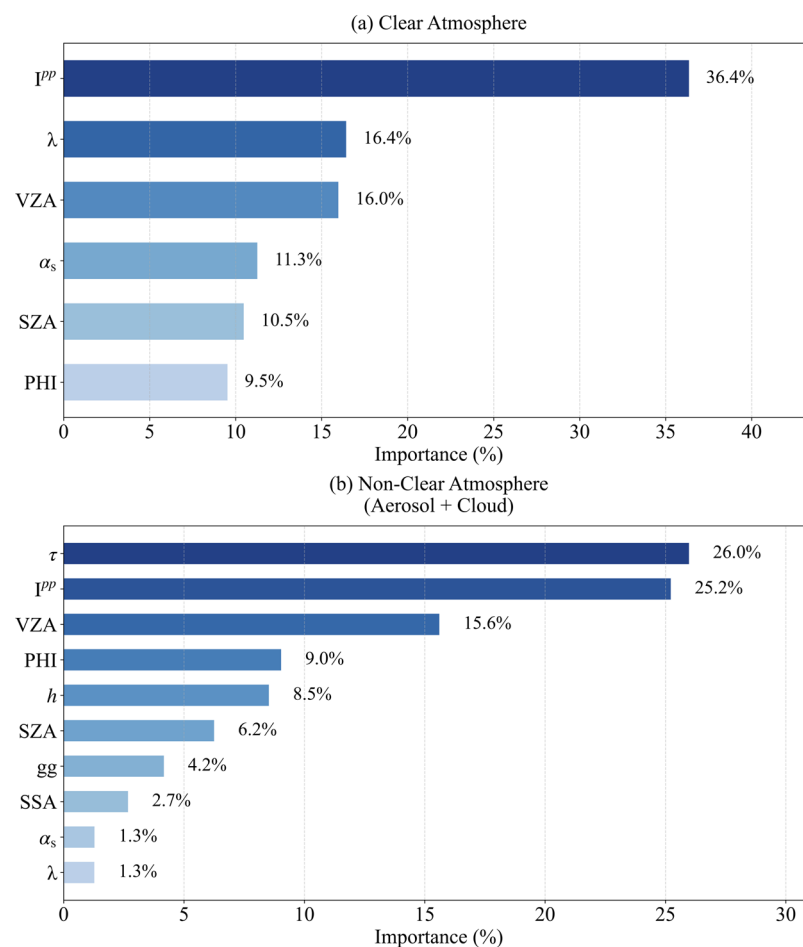


Figure 8. Importance ranking of the six features under (a) clear sky atmosphere, and ten features under (b) non-clear sky atmosphere.

5. Discussion

The XGBoost model is primarily trained and validated for the total intensity I under specific atmospheric setups. While this model demonstrates high accuracy and efficiency within this domain, some inherent limitations remain to be addressed. For example, the current dataset does not cover a wider range of atmospheric profiles or aerosol and cloud types. Specifically, the aerosol types considered in this study do not include mineral dust. Consequently, the present model should not be applied directly to dust-dominated atmospheric conditions. Mineral aerosols exhibit substantial variability in particle size, mineral composition, absorption, and nonspherical scattering phase functions, which cannot be fully represented by a single generic dust configuration or by the asymmetry factor alone. Furthermore, the dataset is also limited to the selected cloud types; only one idealized configuration of cirrus clouds is included, without covering other ice clouds and mixed-phase clouds. In addition, the current simulations only consider single-layer clouds with a fixed vertical interval of 1 km, whereas multi-layer cloud scenarios feature more complex vertical structures and radiative interactions, which deserve further investigation in future studies. Furthermore, the temperature, pressure, and relative humidity were not independently varied; their individual effects cannot be separated and are only implicitly represented by the prescribed atmospheric profiles, optical properties, and plane-parallel radiance. In particular, the use of aerosol optical properties at a fixed relative humidity of 50% limits the model's applicability under strongly varying humidity conditions. In realistic atmospheric environments, fluctuating humidity significantly alters the particle size and optical properties of hydrophilic aerosols, which in turn influences the radiative transfer processes. Because our dataset relies on prescribed humidity conditions, such humidity-induced aerosol hygroscopic growth is not explicitly represented. These limitations restrict the current conclusions to the atmospheric conditions and parameter ranges covered by the training dataset. Future extensions will explicitly sample meteorological profiles and incorporate multiple mineral-dust modes, additional cloud microphysical types, and humidity-dependent aerosol optical properties.

Beyond the total intensity I , extending the machine learning framework to calculate the linear polarization intensity Q represents a vital progression for complete radiative transfer modeling. To investigate the potential relationship and ratio behavior between Q and I , this study compiled a dedicated dataset comprising 70 samples under clear and clean atmospheric scenarios. For each sample, the four-dimensional Stokes vector radiances (I, Q, U, V) were simulated at a representative wavelength of 450 nm, with SZA ranging from 0° to 89° , VZA ranging from 0° to 79° , and a fixed surface albedo of 0.2. Existing data show that as the zenith angle increases, the ratio between the Q/I values under I^{PP} (Q^{PP}/I^{PP}) and those under I^{SS} (Q^{SS}/I^{SS}) fluctuates more significantly (Figure 9).

Therefore, this study attempts to address clean and clear-sky atmospheric conditions by incorporating Q^{PP}/I^{PP} as an influencing factor and adding the target variables Q^{SS}/I^{SS} to obtain the Q^{SS} , thereby enabling the calculation of radiation polarization. The new XGBoost prediction model shows that the R^2 value for the target variable Q^{SS}/I^{SS} is 0.9975, exploring the feasibility of the model for calculating radiation polarization. However, considering that aerosol and cloudy atmospheres have more influencing factors, we need to consider additional factors in the future to continuously refine this model to meet the requirements of various atmospheric conditions.

A further limitation is the assumption of Lambertian surface reflection. Under large solar or viewing zenith angles, surface BRDF effects may introduce substantial angular variations in top-of-atmosphere radiance and interact with atmospheric curvature effects. Future datasets should therefore include representative BRDF models and parameters to extend the model to anisotropically reflecting land surfaces.

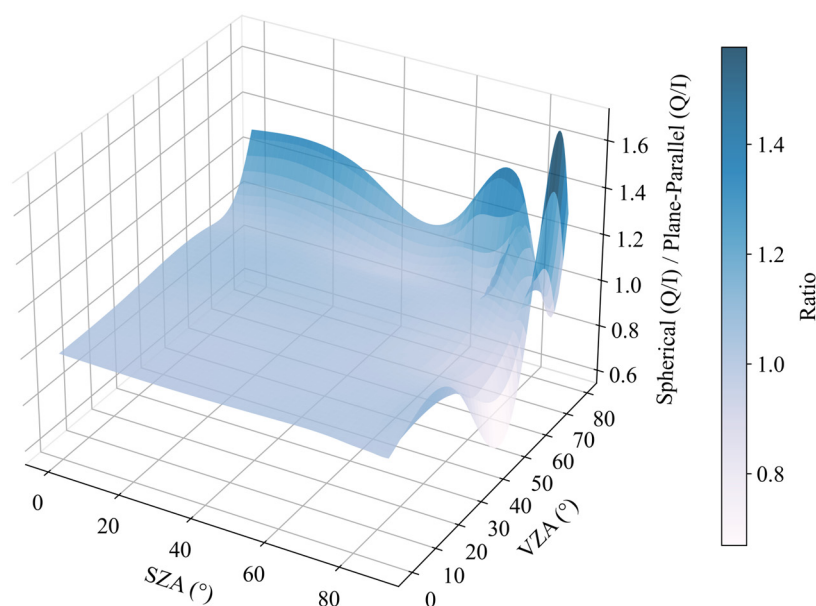


Figure 9. Plot of the ratio between Q^{PP}/I^{PP} and Q^{SS}/I^{SS} at a wavelength of 450 nm as a function of SZA and VZA.

In addition, as a data-driven method, the model may be unreliable when extrapolated beyond the atmospheric, angular, and spectral ranges represented in the training dataset. The Monte Carlo reference radiances also contain residual statistical noise arising from finite photon sampling, which may propagate into model training and evaluation. Before practical application, the model should therefore be further validated against independent high-fidelity radiative transfer simulations and real satellite observations, with particular attention to out-of-domain conditions and reference-data uncertainty.

6. Conclusions

This study establishes a mapping model based on XGBoost machine learning, achieving high-precision and high-efficiency conversion from I^{PP} to I^{SS} , providing a new approach to solving the problems of high computational complexity and poor timeliness in traditional spherical atmospheric radiative transfer calculations. Firstly, this method achieves a significant improvement in computational efficiency. Compared to the Monte Carlo physical model, this approach increases the computational efficiency by approximately 285 times for the same data volume. This benchmark was achieved by evaluating the entire comparison dataset with a batch size of about 3500 samples on an Intel Core i5-10200H CPU using multi-threaded parallel processing, matching the hardware environment utilized for the Monte Carlo simulations. Secondly, it delivers a breakthrough in the accuracy of large-angle radiation correction. Compared with the plane-parallel model and pseudo-spherical model, the proposed model substantially reduces radiation biases arising from spherical geometric effects by incorporating enhanced training with large-angle samples. Overall, the XGBoost model significantly outperforms the traditional approximation, reducing mean error to $4.06 \text{ W m}^{-2} \text{ sr}^{-1} \text{ nm}^{-1}$ and standard deviation to $8.19 \text{ W m}^{-2} \text{ sr}^{-1} \text{ nm}^{-1}$, with this improvement remaining critical even under extreme angular conditions ($\text{SZA or VZA} \geq 75^\circ$). In addition, when applied to 300 clear-sky atmospheric simulation cases, the traditional method fails due to large MAPE values, whereas the XGBoost model maintains robust predictive accuracy, yielding a MAPE of approximately 4.64%. Regardless of whether the atmosphere is clear or laden with aerosols and clouds, I^{PP} consistently serves as the most dominant influencing factor, maintaining a stable contribution of 26.6% in both scenarios. This underscores that I^{PP}

provides a fundamental baseline for spherical radiation predictions across many conditions and the model dynamically adjusts its sensitivity to other physical parameters depending on the specific atmospheric state.

This model provides a novel approach for atmospheric correction of satellite remote sensing data and demonstrates the immense potential of machine learning in addressing complex physical problems by bridging simplified models with real physical processes through data-driven approaches. The developed XGBoost mapping model establishes a foundational framework for transforming plane-parallel radiative calculations into accurate spherical radiation. Future research can further investigate a wide range of atmospheric profiles, even those representing extreme atmospheric conditions, since incorporating meteorological parameters such as temperature–pressure profiles may help quantify their nonlinear effects on spherical radiative transfer paths.

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Abbreviations

The following abbreviations are used in this manuscript:

ARE	Absolute Relative Error
gg	Asymmetry Factor
<i>h</i>	Central Height of Aerosol/Cloud Layer
<i>I</i>	Total Intensity
IPSS	Improved Pseudo-Spherical Scheme
LIDORT	Linearized Discrete Ordinate Radiative Transfer
MAPE	Mean Absolute Percentage Error
MERSI-III	Medium Resolution Spectral Imager-III
MYSTIC	Monte Carlo Code for the Physically Correct Tracing of Photons in Cloudy Atmospheres
OPAC	Optical Properties of Aerosols and Clouds
<i>PHI</i>	Azimuth angle
PSS	Pseudo-Spherical Scheme
<i>Q</i>	Linear Polarization Intensity (Stokes parameter <i>Q</i>)
<i>R</i> ²	Coefficient of Determination
RMSE	Root Mean Square Error
SOOT	Black Carbon

SSA	Single Scattering Albedo
SSCM	Sea Salt Coarse Mode
SUSO	Soluble sulfate aerosols
SZA	Solar Zenith Angle
VLIDORT	Vector Linearized Discrete Ordinate Radiative Transfer
VZA	Viewing Zenith Angle
WASO	Water-Soluble Aerosols
XGBoost	Extreme Gradient Boosting

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