

Article

Retrieval of Ozone Profiles from Limb Scattering Measurements of the OMS on FY-3F Satellite

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Highlights

What are the main findings?

- The study presents the first successful retrieval of stratospheric ozone profiles (18–55 km) from the Fengyun-3F satellite's Ozone Monitoring Suite–Limb (OMS-L), China's first UV-Vis hyperspectral limb sounder, using a novel method combining UV wavelength pairing and the Weighted Multiplicative Algebraic Reconstruction Technique (WMART).
- The retrieved OMS-L ozone profiles show good consistency with the established OMPS/LP v2.6 satellite product, with differences generally within 10% between 20 and 50 km, demonstrating the high quality and reliability of the new OMS-L data.

What are the implications of the main findings?

- This work validates OMS-L as a new, high-vertical-resolution data source for stratospheric ozone, enhancing global monitoring capabilities and providing crucial data for atmospheric chemistry and climate change research.
- The successful retrieval contributes significantly to the global effort of stratospheric ozone layer assessment and trend analysis.



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Abstract

The Ozone Monitoring Suite–Limb (OMS-L) carried by the Fengyun-3F (FY-3F) satellite, as China's first effective payload using the limb observation mode to conduct hyperspectral atmospheric detection in the ultraviolet (UV) and visible (Vis) bands, was successfully launched on 3 August 2023. It mainly serves the research in the fields of climate change, atmospheric chemistry, and atmospheric environment. This study is the first to conduct the retrieval of the ozone profiles from OMS-L data. The retrieval scheme utilizes the radiances within the UV band, normalizing them to the radiance at the upper tangent height. To minimize the impact of aerosol scattering, the pair method is implemented, with seven carefully selected wavelength pairs fully exploiting ozone's UV absorption characteristics. The weighted multiplicative algebraic reconstruction technique (WMART) is then applied to effectively integrate multi-wavelength information, in tandem with an iterative retrieval process using the radiative transfer model. This approach yields ozone concentration profiles in the altitude range of approximately 18–55 km. The retrieval errors resulting from the parameters are estimated to be 5–13% above 25 km, increasing to 10–30% in the upper troposphere. Comparison of OMS-L retrieved ozone profiles with the OMPS/LP v2.6 product reveals good consistency, with differences generally within 10% in the

20–50 km altitude range. However, biases are more pronounced at lower altitudes, particularly in tropical regions. This work conclusively demonstrates that OMS-L can accurately measure stratospheric ozone profiles with high vertical resolution, thereby contributing significantly to the field of atmospheric science.

Keywords: ozone profile; limb sounding; retrieval; OMS-L; OMPS/LP

1. Introduction

Atmospheric ozone, a crucial component of Earth's atmospheric composition, plays an irreplaceable role in both ecological and climate systems [1]. Stratospheric ozone can effectively absorb the majority of solar ultraviolet (UV) radiance, thereby shielding terrestrial life from harmful exposure and helping maintain planetary ecological balance [2,3]. While substantial progress has been made in understanding the chemistry of stratospheric ozone, there are still many issues that urgently need to be clarified in aspects such as the recovery of the ozone hole [4,5], the impact of increasing greenhouse gases on atmospheric circulation and temperature [6], the interaction between stratospheric and tropospheric ozone [7,8], and the long-term trend of ozone [9].

Recent studies underscore the complexity of ozone layer dynamics. For instance, Kessenich et al. comprehensively analyzed the monthly and daily ozone variations at different altitudes and latitudes within the Antarctic ozone hole and found that although there were signs of recovery in early spring, the ozone in the middle stratosphere in October has continued to decrease significantly since 2004, highlighting the importance of continuous monitoring and evaluation of the ozone layer [10]. Ardra et al. found unprecedented ozone depletion during the winter and spring seasons in the Arctic in recent years [11]. Ma et al. revealed a new mechanism of stratospheric ozone depletion—the smoke charging vortex caused by wildfires through advanced numerical simulations and satellite observations [12]. Chen et al. quantified for the first time the stratospheric intrusion to the surface (SITS) event using data from ground-based air monitoring stations in China, and analyzed the long-term and short-term effects of stratospheric ozone on the evolution of ground-level ozone concentration in China [13]. Therefore, accurately understanding the vertical distribution of stratospheric ozone is of great value for a deeper understanding of the operating mechanism of the Earth's ecological system, evaluating the impact of climate change on the ecological environment, and formulating effective environmental protection strategies.

Research on the spatiotemporal distribution of atmospheric ozone relies on ground-based monitoring [14], model simulation [15], and satellite remote sensing measurements [16]. Compared with ground-based monitoring methods and chemical transport models, satellite remote sensing observation has the advantages of wide coverage, high spatial resolution, and a long time series. The limb-sounding technique, which is widely used in recent satellite instruments, combines the advantages of nadir observation and occultation mode. It has a better vertical resolution compared to the nadir geometry and a higher horizontal sampling rate than occultation measurements [17]. Limb-sounding techniques can be classified into limb emission and limb scattering. The former often suffers from a low signal-to-noise ratio due to weak atmospheric emission, while the latter relies on scattered solar radiation and is thus restricted to daytime measurements [18].

A new generation of limb-scattering instruments has been launched by various countries at home and abroad, including the Scanning Imaging Absorption Spectrometer for Atmospheric Cartography (SCIAMACHY) [19], the Optical Spectrograph and Infrared Imager

System (OSIRIS) [20], the Ozone Mapper and Profile Suite Limb Profiler (OMPS/LP) [21], the Ozone Monitoring Suite–Limb (OMS-L) [22], and the Backward Limb Spectrometer (BLS) [2]. These sensors provide high-vertical-resolution (1–3 km) ozone profiles with global coverage by measuring scattered sunlight.

The Fengyun-3F (FY-3F) satellite, a key component of China’s second-generation polar-orbiting Fengyun-3 meteorological series, was successfully launched on 3 August 2023, and has since operated in stable condition. Among its payloads is the Ozone Monitoring Suite–Limb (OMS-L), a newly developed sensor designed for trace gases observation, including ozone profile retrieval. OMS-L employs a limb-sounding technique combined with continuous spectral measurement, which is applied for the first time, significantly improving both spectral and spatial resolution. A novel retrieval scheme is developed for retrieving the stratospheric ozone profiles from OMS-L measurements. The method uses UV wavelength pairing and the weighted multiplicative algebraic reconstruction technique (WMART), and in combination with the radiative transfer model, to retrieve ozone profiles at altitudes ranging from ~18 to 55 km. Moreover, the retrieval results from OMS-L are compared with the OMPS/LP v2.6 ozone profile product. The purpose of this study is to deeply explore the methods and technologies for retrieving the stratospheric ozone profile from OMS-L data, and rigorously evaluate the accuracy and reliability of the retrieval results.

2. Materials and Methods

2.1. Materials

2.1.1. The OMS-L on FY-3F Satellite

The FY-3F satellite is a morning-orbit, sun-synchronous polar satellite designed for continuous optical and microwave imaging as well as vertical sounding of the land–atmosphere system. It operates at an average altitude of approximately 836 km, with an orbital inclination of about 98.8°, and a descending node local time between 10:00 and 10:20. The orbital period is approximately 101.5 min.

The FY-3F satellite carries ten powerful and advanced remote sensing instruments (Figure 1a). Among them, the OMS-L is a newly developed payload and represents China’s first operational limb-sounding instrument dedicated to hyperspectral atmospheric detection across the ultraviolet and visible (UV–Vis) bands (290–500 nm). OMS-L is a spectrometer based on a double-dispersion system (prism plus grating) and uses a cooled two-dimensional Complementary Metal–Oxide–Semiconductor (CMOS) detector for imaging. Key instrument performance parameters are summarized in Table 1. Incoming scattered radiance is first separated by a Brewster-angle polarizer into partially polarized and linearly polarized components. The partially polarized light is subsequently split via a beam splitter and imaged onto two CMOS detector arrays, generating spectral data in two bands used primarily for atmospheric detection. The linearly polarized component is directed to a third CMOS array, providing data for polarization correction of the first two bands [22].

The OMS-L instrument employs the limb-sounding technique to observe scattered solar radiation in the ultraviolet and visible (UV–Vis) spectral range from the stratosphere. This enables the retrieval of vertical profile data for various trace gases—including global O₃, NO₂, SO₂, BrO, HCHO, and OCIO—as well as quantitative and qualitative products related to aerosols and clouds. In the limb observation geometry, the location where the instrument’s line of sight (LOS) reaches its minimum distance to the Earth’s surface is defined as the tangent point (TP). The altitude of the TP, after correction using a digital elevation model (DEM), is referred to as the tangent height (TH). A schematic illustration of the limb observation geometry is provided in Figure 1b.

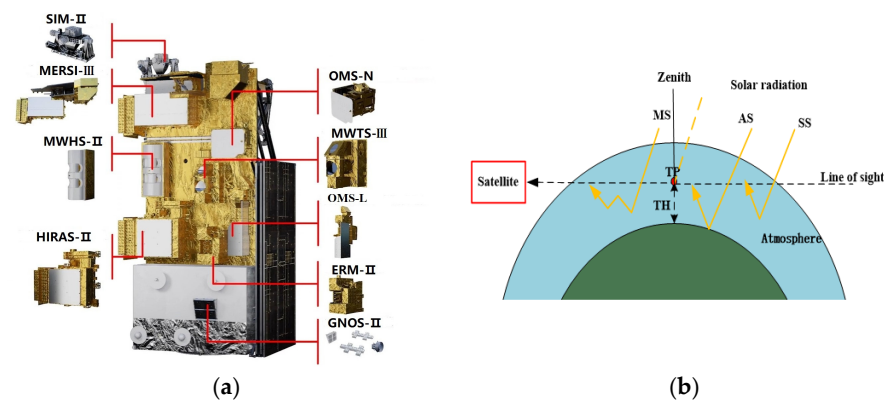


Figure 1. (a) Remote sensing instruments carried by FY-3F satellite (adapted from NSMC website [23]). (b) Schematic diagram of the viewing geometry of a satellite limb observation, showing the tangent point (TP) and the tangent height (TH), (SS: single scatter, AS: albedo scatter, MS: multiple scatter). [24].

Table 1. Several main instrument performance indicators of OMS-L [22].

Item	Indicator
Spectral coverage	290–500 nm
Spectral resolution	0.6 nm
SNR	$>300@0.1 \mu\text{W}/(\text{cm}^2 \times \text{sr} \times \text{nm})$
Vertical coverage	15–60 km
Vertical resolution	3 km
Instantaneous field of view	2.3° (horizontal) $\times$ 0.045° (vertical)

2.1.2. The OMS-L Level-1 Version 1.2 Data

The OMS-L Level 1 version 1.2 (L1 v1.2) product provides calibrated radiometric spectra derived from a sequence of processing steps applied to the raw L0 data and static auxiliary inputs. These steps include data decoding, geolocation, bad-pixel detection, dark-current processing, spectral calibration, radiometric calibration, polarization correction, and quality control [22]. Notably, the Level-1 processing incorporates comprehensive stray-light and polarization corrections. Stray light is characterized and corrected, with the post-correction residual error typically maintained below 2% in the core UV spectral range used for ozone retrieval. For polarization correction, OMS-L utilizes a dedicated optical design featuring a Brewster angle polarizer to split incoming radiance. A specialized algorithm then applies polarization correction coefficients—derived from measurements in the dedicated polarization channel (Band 3)—to Bands 1 and 2, effectively mitigating polarization sensitivity. The residual error after polarization correction is estimated to be below 1%. These performance estimates are based on pre-launch calibration and ongoing on-orbit validation.

Figure 2a shows the available OMS-L observation orbits on 1 August 2024, with the red arrow indicating the satellite's flight direction. Due to its orbital inclination of approximately 98° , the instrument achieves near-global coverage, sampling latitudes between 80°S and 80°N . The satellite completes 14–15 orbits per day, with roughly 135 limb scans per orbit. Figure 2b presents sample tangent heights (THs) measured during an orbit at 00:47 UTC on the same day. The sensor observes 15 discrete TH layers per scan; however, the TH scanning range is not fixed. It varies with latitude, generally covering lower altitudes in tropical regions and toward the end of an orbital scan. As a result, the retrieval altitude range also varies geographically.

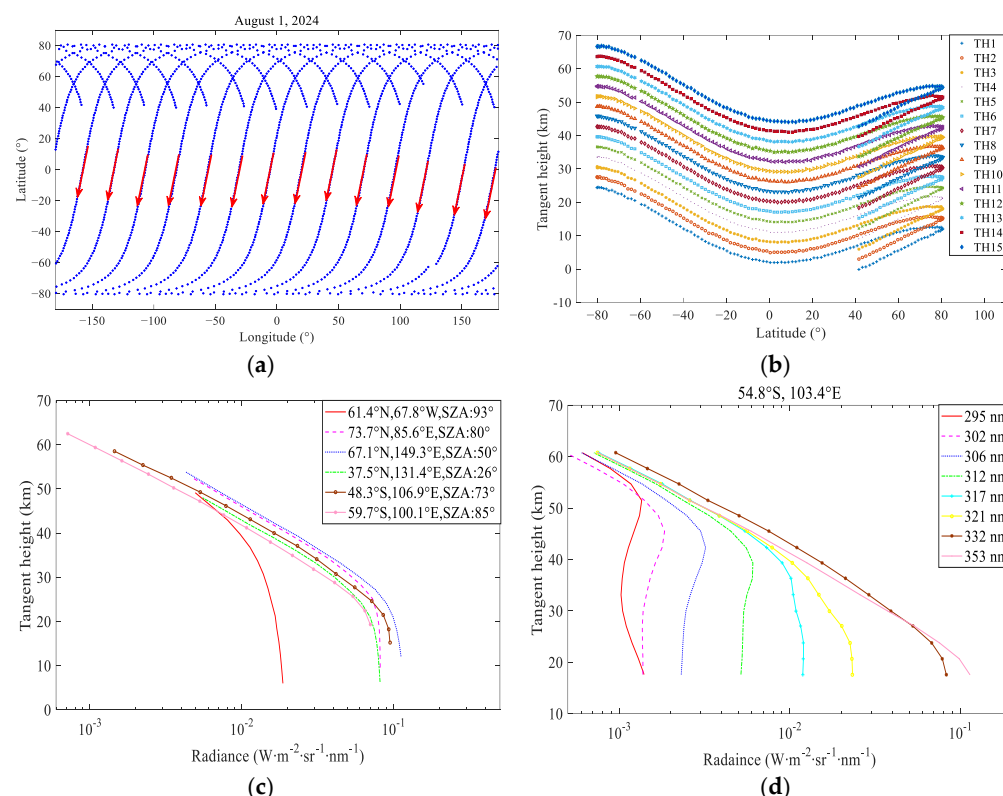


Figure 2. (a) OMS-L daily orbits and observation geometry sketch, red arrows indicate the satellite flight direction. (b) Sample THs measured by OMS-L during the orbit at 00:47 on the same day. (c) Distribution of limb radiance profiles at a wavelength of 332 nm for different latitudes on the same orbit. (d) Sample set of OMS-L limb radiance profiles for ozone retrieval.

Figure 2c displays radiance profiles at 332 nm for the same orbit across different latitudes, plotted as a function of TH. Slight differences in both radiance magnitude and altitude coverage are evident across latitudes. Radiance is weaker at the beginning and end of orbital scans due to larger solar zenith angles (SZA). In high-latitude regions, radiance at lower altitudes is strongly influenced by atmospheric absorption and scattering. Figure 2d shows sample limb radiance profiles at selected wavelengths within the Hartley–Huggins band. To accommodate the decreasing ozone absorption cross-section at longer wavelengths, measurements at lower altitudes are prioritized in those spectral regions. In the UV band, Rayleigh scattering and trace gas absorption cause the limb radiance to reach a maximum at a specific altitude. The tangent height below which the radiance profile remains nearly constant is referred to as the “knee,” representing the minimum detectable altitude for a given wavelength.

2.1.3. Forward Model and a Priori Data

In this study, the radiative transfer model for SCIAMACHY (SCIATRAN) is employed as the forward model to calculate the simulated limb radiances for retrieval purposes. The forward model comprehensively accounts for the phenomenon of multiple scattering and resolves the scattered light within a spherical atmospheric geometry [25]. In the absence of the polarization effect, the discrete ordinate method (DOM) is utilized to solve the radiative transfer equation, while also incorporating the effect of atmospheric refraction. Ozone is considered the primary absorbing gas in the model. The ozone absorption cross-section at 223 K, as provided by Bogumil et al. [26], is adopted.

The temperature, pressure, and a priori ozone profiles used in the retrieval procedure of this work are all sourced from the built-in database of SCIATRAN. These profiles,

provided by the McLinden climatology (C. McLinden, Meteorological Service of Canada, private communication), contain the monthly and latitude dependent vertical distributions of O₃, NO₂, BrO, and OClO volume mixing ratios, along with pressure and temperature in the altitude region between 0 and 100 km. The volume mixing ratio of ozone can be converted into ozone number density based on the temperature and pressure. The vertical sampling interval of the a priori profiles in SCIATRAN is 1 km; consequently, the vertical resolution of the retrieved profiles in this study is 1 km. Theoretically, any reasonable profile can serve as an a priori profile. However, different initial profiles yield different retrievals.

In this study, the surface albedo is fixed at a constant value of 0.5, and the impact of clouds is deliberately excluded. The LOWTRAN [27,28] aerosol type in SCIATRAN is adopted, with the stratospheric aerosol loading assigned to the background.

2.2. Methods

The method utilized in this study to retrieve the vertical distribution of ozone concentration from OMS-L measurements adheres to the approach proposed by Zhu et al. [19] for obtaining ozone profiles from SCIAMACHY limb scattering measurements in the Hartley–Huggins band. This retrieval technique is similar to the one employed by Degenstein et al. [29], both of methodologies utilize retrieval vectors that exhibit a positive correlation with ozone concentration variations.

2.2.1. Retrieval Vector

The ozone absorption cross-section is characterized by high absorption peaks in both the UV and Vis bands. However, according to the specifications of the OMS-L L1 v1.2 data, its spectral band is applicable to the retrieval of ozone profile in the UV band. Consequently, in this study, the measured values of Channel 1 (287.2–402.3 nm), which has a spectral resolution of 0.4–0.44 nm, are employed for the retrieval process. In the Hartley–Huggins band, the ozone absorption and Rayleigh scattering cross-sections vary rapidly. As emphasized by Rohen et al. [30], the selection of appropriate wavelength is therefore critical. The retrieval absorption wavelengths and a reference wavelength were determined based on the altitude at which ozone is most sensitive at different wavelengths. Therefore, the sensitivity of the limb radiance at different wavelengths to ozone number density is calculated, which is known as the limb radiance weighting function or Jacobian matrix [2], and is expressed as:

$$\mathbf{K} = \frac{\partial I(\lambda, H_j)}{\partial [\text{O}_3]_i} = \frac{\Delta I(\lambda, H_j)}{\Delta [\text{O}_3]_i} \quad (1)$$

where $I(\lambda, H_j)$ denotes the radiance at the j th TH (H_j) for the wavelength λ , and $[\text{O}_3]_i$ represents the ozone number density at the i th atmospheric altitude. Figure 3, calculated by SCIATRAN, illustrates the peak sensitivity of the limb radiance at selected wavelengths to ozone at different altitudes, under specific observation conditions, with a 10% perturbation in the ozone concentration. As depicted in Figure 3, the weighting function reaches a peak value as the altitude increases, indicating that wavelengths within this range are highly sensitive to ozone variations. The weighting functions for strong-absorption wavelengths are larger than those for weak-absorption wavelengths. This indicates that at wavelengths with stronger ozone absorption, the radiance decreases more significantly as ozone concentration increases. In the UV band, as the wavelength increases, photons can penetrate to lower altitudes due to the reduced absorption by ozone. Generally, the UV band is most sensitive to ozone above 20 km.

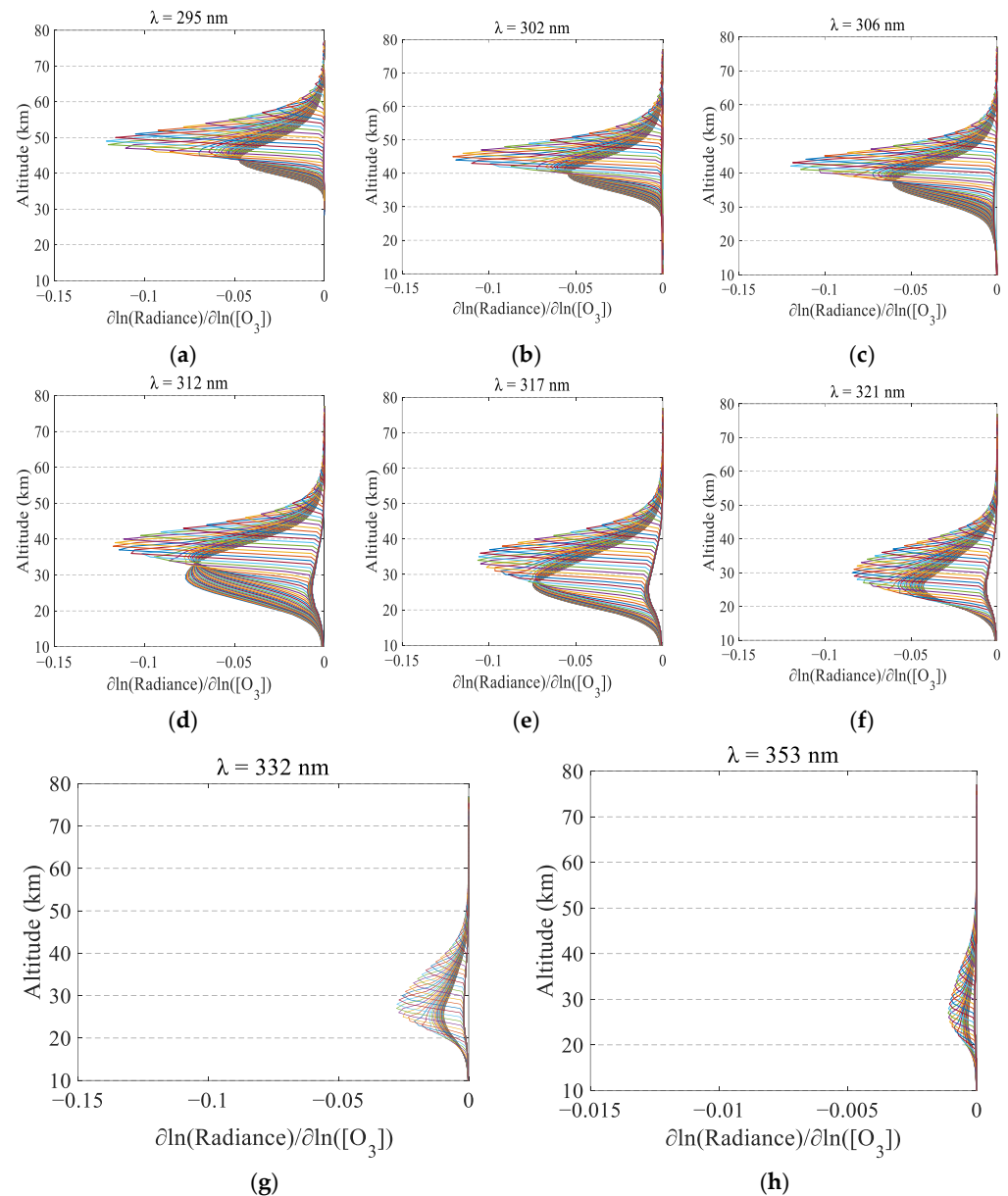


Figure 3. The sensitivities of the limb radiance calculated by SCIATRAN at selected wavelengths to ozone number density at different altitudes, under the given observation conditions (the SZA is 60° ; the relative azimuth angle is 90°). (a) 295 nm; (b) 302 nm; (c) 306 nm; (d) 312 nm; (e) 317 nm; (f) 321 nm; (g) 332 nm; and (h) 353 nm.

To reduce the effects of instrument calibration errors and scattered light from the lower atmosphere, the limb radiance profile at each wavelength is normalized at a relatively higher TH. The elevated TH, referred to as the reference TH, corresponds to an altitude at which the radiance at that wavelength is largely insensitive to ozone absorption [31]. As indicated by the limb radiance weighting function, each wavelength exhibits peak sensitivity to ozone variations at a distinct altitude. Therefore, the radiance for each wavelength is normalized using its own reference TH, as summarized in Table 2. The normalization is performed according to the following equation:

$$I_N(\lambda, H) = \frac{I(\lambda, H)}{I(\lambda, H_{\text{ref}})} \quad (2)$$

where $I_N(\lambda, H)$ represents the normalized radiance at wavelength λ , while $I(\lambda, H_{\text{ref}})$ is the measured radiance at the reference TH (H_{ref}). The reference TH for each wavelength pair (Table 2) was selected to be sufficiently high such that the radiance at that altitude is largely insensitive to ozone absorption. This approach effectively removes common-mode errors, including those from instrument calibration and Rayleigh scattering.

Table 2. Definitions of the 7 pairs calculated from the measured limb radiances.

	HPV1	HPV2	HPV3	HPV4	HPV5	HPV6	HPV7
λ_{abs} (nm)	295	302	306	312	317	321	332
λ_{ref} (nm)	353	353	353	353	353	353	353
H_{min} (km)	49	42	42	36	33	27	18
H_{max} (km)	57	54	51	49	42	40	36
H_{ref} (km)	60	60	54	52	45	42	40

Secondly, the absorption range of the Hartley–Huggins band spans from 200 to 300 nm. The shorter wavelength segment of this band overlaps with the absorption band of oxygen molecules. Hence, as noted by Roth et al. [32], there can only be one reference wavelength for wavelength pairing within the Hartley–Huggins band. A series of discrete wavelengths, carefully selected to circumvent Fraunhofer lines and minimize scattered light interference, are paired with a wavelength that is insensitive to ozone. Once paired, these wavelength combinations maintain identical sensitivities to ozone concentration changes. This study follows the methodology proposed by Degenstein et al. [29] and defines the wavelength pairing within the Hartley–Huggins band to construct the retrieval vector, namely the Hartley pairing vector (HPV), denoted as y_p :

$$y_p(\lambda, H) = \frac{I_N(\lambda_{\text{ref}}, H)}{I_N(\lambda_{\text{abs}}, H)} \quad (3)$$

where λ_{ref} represents the reference wavelength, and λ_{abs} represents the absorption wavelengths. The HPV is a function of altitude and increases with the ozone concentration. The retrieval vector developed through the pairing approach can effectively minimize the impact of inaccurate estimations of Rayleigh scattering and stratospheric aerosols on the retrieval results [19]. The performance of the forward model in simulating the HPVs is critical for the retrieval. To validate this, we compared the observed and simulated HPVs across a wide range of conditions. As shown in Supplementary Figure S1, which presents representative cases from high, mid, and low latitudes, the forward model successfully reproduces the observed HPVs across various wavelengths and tangent heights. The corresponding residuals are small and random, demonstrating good consistency between the measurement and simulation.

In this study, absorption wavelengths of 295, 302, 306, 312, 317, 321, and 332 nm are paired with the reference wavelength of 353 nm to retrieve the ozone profiles in the upper-middle stratosphere (18–55 km), as shown in Table 2.

2.2.2. Weighted Multiplicative Algebraic Reconstruction Technique

For the iterative of the ozone profile in this study, the weighted multiplicative algebraic reconstruction technique (WMART) proposed by Degenstein et al. [29] is employed. This technique has been applied to the retrieval of ozone profiles from OSIRIS measurements, and its iterative formula is as follows:

$$x^{n+1} = x^n \mathbf{W}^{\text{pair}} \frac{y_p^{\text{obs}}}{y_p^{\text{mod}}} \mathbf{W}^{\text{LOS}} \quad (4)$$

where x^n denotes the ozone profile x at the n th iteration. y_p^{obs} and y_p^{mod} represent the observed retrieval vector and the modeled retrieval vector, respectively. $\mathbf{W}^{\text{LOS}}$ corresponds to the line-of-sight weighting factors, which indicate the influence weight of the TH or LOS on the retrieval altitude. $\mathbf{W}^{\text{pair}}$ refers to the wavelength weighting factors, which reflect the significance of the wavelength pairs for each altitude. At each altitude, the sum of the line-of-sight weighting factors along the LOS and the sum of the wavelength weighting factors across all wavelengths are both equal to 1.

The WMART algorithm iteratively updates the atmospheric state parameters using the ratios of the elements of the observed and modeled vectors. The ability of retrieving ozone at a certain altitude using multispectral information is not exclusive to the WMART. Nevertheless, it is essential for integrating multi-wavelength information within the Hartley–Huggins absorption band. For simplicity, only three lines of sight are considered for each altitude. $\mathbf{W}^{\text{LOS}}$ was set according to the geometry of the limb view, giving higher weights to tangent heights closer to the retrieval altitude, as in Zhu et al., [17], thus it will not be described in detail here. In WMART algorithm, the wavelength weighting factors ($\mathbf{W}^{\text{pair}}$) define the relative contribution of each HPV to the altitude. The contribution of each HPV changes gradually within an altitude range to mitigate the oscillations in the retrieved profiles. These oscillations are caused by small systematic errors that vary with wavelength and altitude in the forward model [29]. Figure 4 shows a graph of the weighting factors assigned to each wavelength pair used in this study. The weighting factor of each pair gradually increases from zero at the lowest altitude to the altitude where it is most significant for retrieving, and then gradually decreases to zero at the highest altitude.

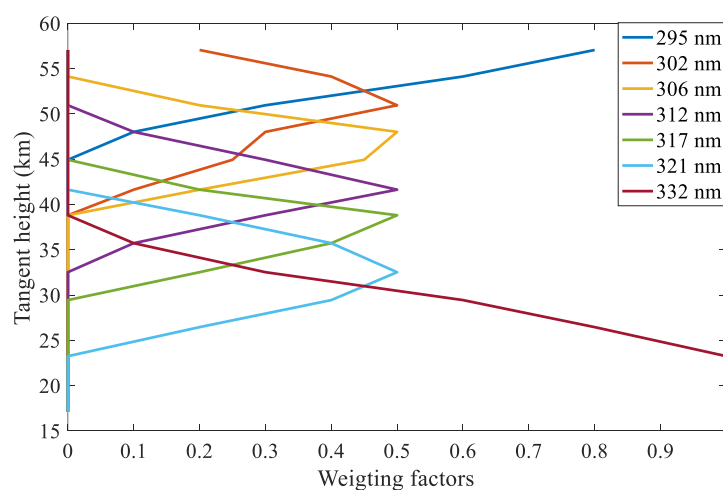


Figure 4. The wavelength weighting factors assigned to each of vectors as a function of altitude.

The WMART algorithm was implemented with a fixed number of 10 iterations for all retrievals presented in this study. This choice was validated through extensive sensitivity tests, which confirmed that the solution is stable and that no significant improvement in accuracy is achieved beyond this point. The convergence behavior and the impact of the iteration count are illustrated in Supplementary Figure S2. No additional Tikhonov regularization was applied.

3. Results

3.1. Sensitivity Analysis

A common framework for appropriately communicating uncertainty and other measurement attributes was proposed by von Clarmann et al. [33], along with a list of suggestions that are expected to contribute to the unification of how retrieval errors are reported.

The existing literature [34,35] has comprehensively discussed the sensitivity analysis of ozone profile retrieval from limb scattering. However, the sensitivity of parameters for ozone profile retrieval using only the UV band differs from that when the UV and Vis bands are combined for use, leading to some distinct outcomes. Several main parameters affecting the retrieval accuracy are discussed below.

The offset of the TH is the primary source of error in extracting the ozone profile from limb radiance [36]. In the OMS-L L1 product, TH values have been determined by satellite attitude and terrain correction. Nevertheless, achieving absolute accuracy in TH remains a challenge. The sensitivity of retrieval results to pointing error is simulated by shifting the data upward or downward by an offset. Figure 5a illustrates the changes in retrieved ozone profiles when TH values are shifted upward or downward by 0.2 km and 0.5 km, respectively. Overall, when the TH offset is approximately 0.2 km, the relative deviation of the retrieval is constrained within 5%. When the TH offset reaches 0.5 km, the maximum deviation exceeds 10%. Generally, TH offset-induced retrieved profiles exhibit vertical displacements in altitude. Notably, the lowest retrieval altitude is around 18 km, and thus, the deviation below this altitude approaches zero.

The WMART equation requires an initial ozone profile, known as the a priori profile. Understanding how the initial guess impacts the retrieval solution is of crucial importance. As per the study by Zhu et al. [35], perturbations in the a priori profile prevent the solution from achieving a high response at the upper and lower boundaries of the retrieval, consequently increasing the deviations within these ranges. Figure 5b shows the variations in retrieved ozone profiles when a priori profiles at different latitudes (75°N, 45°N, 5°N, 45°S, and 75°S) in the same month are respectively used as initial guesses for the retrieval along the same orbit. It is assumed that the profile retrieved with the a priori guess at 5°N is the true result, while the others are not. Overall, all deviations are relatively large at the retrieval boundaries, and the retrieval discrepancies increase as the differences in the a priori profiles grow.

Although normalization can reduce most of the effects of surface albedo and clouds, these effects cannot be completely eliminated [37]. The sensitivity of the retrieved ozone profile to surface albedo was simulated and analyzed, and the results are shown in Figure 5c. Surface albedo mainly affects the retrieval of the ozone profile below 40 km. Owing to radiance normalization and the use of UV wavelengths, its impact is not significant. Assuming the true albedo is 0.5, when the albedo is set to 0.9, the maximum error at 20 km may exceed 1%. In the Hartley–Huggins band, due to increased ozone absorption and a higher scattering height, the effect of albedo diminishes, which benefits the retrieval of ozone in the upper-middle stratosphere.

Although UV radiance is less sensitive to the perturbation in the aerosol extinction profile, aerosols remain one of the most significant sources of systematic errors in stratospheric ozone concentration retrieval. It is assumed that a moderate volcanic event occurs in the stratosphere, during which the stratospheric aerosol extinction coefficient is several times that of the background load [2]. In this study, the sensitivity of ozone profile retrieval to aerosol extinction coefficients of different multiples was simulated and analyzed, with the results shown in Figure 5d. The maximum deviation occurs at an altitude of 20 km. When the aerosol extinction profile is halved, the retrieved ozone concentration is lower than normal, with the maximum deviation reaching 5%. When the aerosol extinction profile doubles or during a moderate volcanic event, the retrieved ozone concentration is higher than normal level, with the maximum deviation reaching 10%.

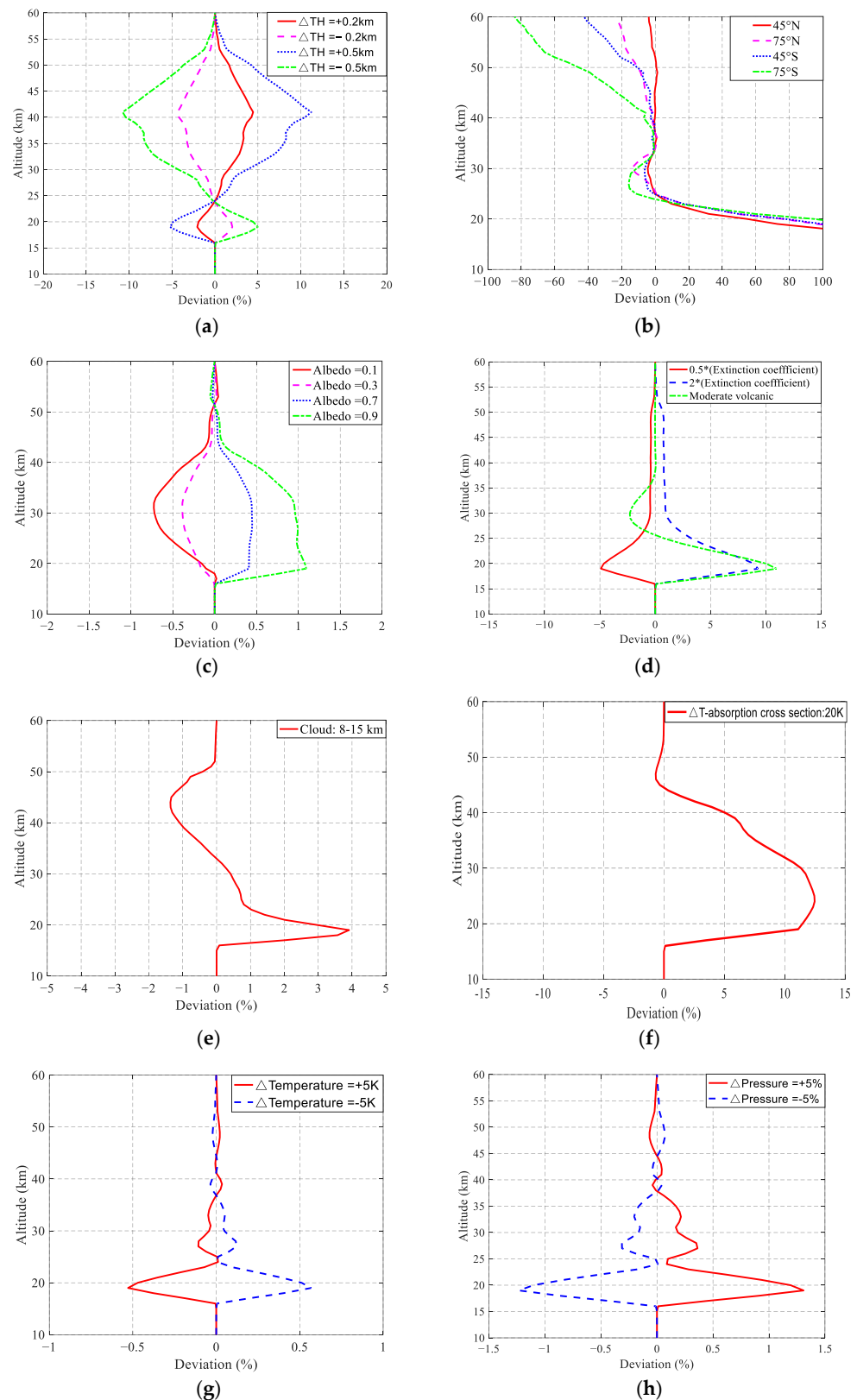


Figure 5. Ozone retrieval deviations caused by parameter inaccuracies. (a) Different TH offsets. (b) A priori profiles at different latitudes. (c) Different surface albedos. (d) Cloud height of 8–15 km. (e) Aerosol extinction profiles with different scaling factors. (f) Ozone absorption cross-sections with a temperature difference of 20 K. (g) Temperature with an increase and decrease range of ± 5 K. (h) Pressure with a scaling factor of $\pm 5\%$.

In this study, clouds were not considered. However, atmospheric clouds play a vital role in the reflection, absorption, and transmission of solar radiation, thereby influencing ozone profile retrieval [38]. When investigating the impact of clouds on the retrievals, the clouds are assumed to be homogeneous both vertically and horizontally. A water cloud with an optical thickness of 5 (@500 nm) and a cloud height ranging from 8 to 15 km is assumed, with an effective radius of water droplets of 6 μm . The deviations in ozone retrieval between cloud-free conditions and the presence of clouds are shown in Figure 5e. The maximum deviation occurs at an altitude of 20 km, approximately 4%. Due to cloud reflection, the ozone concentration in the lower atmosphere is higher, while that in the upper atmosphere is lower due to the influence of the lower-level concentration. Generally, neglecting the influence of clouds on ozone profiles retrieval is essentially similar to the effect of surface albedo in that it increases the reflected solar radiance. Therefore, if tropospheric clouds are ignored or inaccurately modeled, it is one of the causes of errors in ozone profiles retrieval.

Since the ozone absorption cross-section depends only on temperature and not on pressure, the influence of the temperature sensitivity of the ozone cross-section on ozone profile retrieval (T-ozone) was investigated. In this study, ozone concentrations retrieved using the ozone cross-section at 223 K were taken as the true state, and the deviation from the ozone concentration retrieved at 243 K is shown in Figure 5f. When a cross-section at a higher temperature is used to retrieve ozone profile, the ozone concentration is overestimated. The maximum deviation occurs at around 25 km, reaching up to 12%. The influence of the ozone cross-section temperature dependence on ozone retrieval is consistent across all wavelengths used in this study.

The atmospheric temperature and pressure profiles used in the retrieval of this study were obtained from the built-in database of SCIATRAN. It is assumed that the temperature uncertainty is ± 5 K. Figure 5g presents the relative ozone errors caused by the ± 5 K temperature uncertainty. A higher (lower) temperature will lead to an underestimation (overestimation) of the ozone concentration. The errors at all altitudes are less than 0.6%. It is assumed that the pressure uncertainty is $\pm 5\%$. Figure 5h shows examples of the relative error distributions for two different scaling factors in pressure. An increase in pressure leads to an overestimation of the ozone concentration. With a pressure uncertainty of $\pm 5\%$, the retrieved ozone in most parts of the atmosphere has an error of less than 1.5%.

Overall, the sensitivity of parameters for retrieving ozone profiles in the upper-middle stratosphere using only wavelengths within the Hartley–Huggins band differs from that in the Vis band. This difference can be ascribed to the fact that certain parameters, such as surface albedo, aerosols, and clouds, predominantly influence profiles below 40 km. Moreover, reflection and scattering effects are relatively weak in the UV band. The discrepancies in ozone profile retrieval caused by TH offsets, a priori profiles, and ozone absorption cross-sections, exhibits similarities to those reported by Zhu et al. [35]. For most parameters, the maximum retrieval deviation due to inaccuracies occurs around 20 km, which is the lower boundary of the retrieval. Conversely, errors at the upper retrieval boundary (altitudes > 50 km) primarily originate from inaccuracies in the a priori profiles. It should be noted that other potential error sources, such as residual errors from stray light (<2%) and polarization correction (<1%), are not included in this total error budget. Their estimated contributions are significantly smaller than the dominant error sources discussed in this section (e.g., tangent height offset, a priori profile) and are therefore considered secondary in this initial retrieval assessment. Additionally, this error budget primarily focuses on systematic uncertainties. The random error component arising from instrument noise is relatively small for OMS-L in the UV band and has not been included here but will be considered in future comprehensive error analyses.

The total error is calculated as the root-mean-square of the average deviations obtained when each parameter reaches its optimal accuracy, as expressed by the following formula:

$$E_{Total} = \sqrt{\frac{1}{N} (E_{prior}^2 + E_{Alb}^2 + E_{Aer}^2 + E_{Pre}^2 + E_{Tem}^2 + E_{T_{Ozone}}^2 + E_{TH}^2 + E_{Cloud}^2)} \quad (5)$$

where E_{prior} represents the mean deviation in ozone retrieval when using mid latitude and low latitude a priori profiles, respectively. E_{Alb} denotes the average deviation for surface albedos of 0.5 and 0.3. E_{Aer} refers to the deviation when the aerosol extinction profiles are at normal level and halved, respectively. E_{Temp} indicates the deviation when the temperature profile varies by 5 K. E_{Pre} represents the deviation when the pressure changes by 5%. $E_{T_{Ozone}}$ is the retrieval deviation of the ozone cross-section at 223 K and 243 K. E_{TH} stands for the deviation when the TH is offset by 0.2 km. E_{Cloud} represents the deviation between the cases with an 8–15 km cloud and without a cloud. Figure 6 shows the calculated total deviation profile. The total retrieval error of the ozone profile is estimated to be in the range of 5–30% from 20 to 55 km. It is important to note that this total error estimation assumes independence among the individual error sources, as their correlations are not yet well characterized for the OMS-L retrieval.

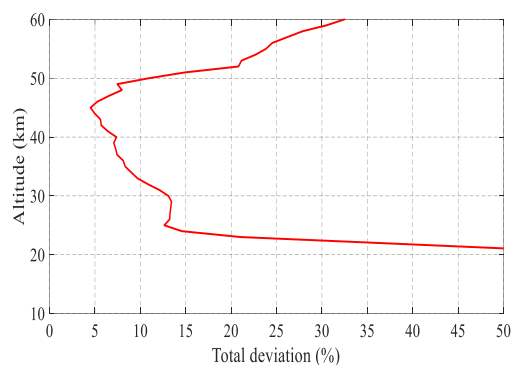


Figure 6. The estimated profile of the total deviation.

The information content and vertical resolution of the retrieval were further characterized by numerically calculating the averaging kernels. The resulting Degrees of Freedom for Signal (DOFS) is typically about 5.6, and the averaging kernels for different latitudes are provided in Supplementary Figure S3, demonstrating good resolution in the 20–50 km range.

Figure 7 presents a representative ozone profile from OMS-L. The error bars at each altitude correspond to the systematic uncertainty derived from the total deviation profile in Figure 6. This illustration allows for an understanding of the confidence in the retrieved values due to forward model and parameter uncertainties.

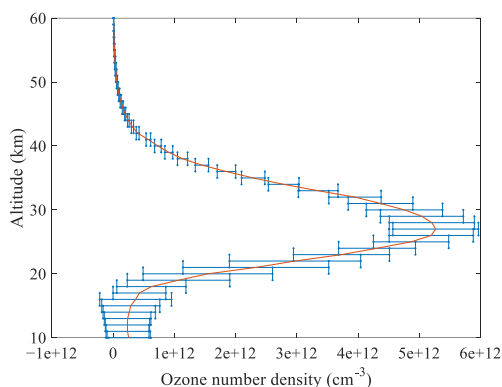


Figure 7. A representative OMS-L retrieved ozone profile with systematic uncertainty, acquired from orbit 0047 at latitude 5.5°N on 1 August 2024.

3.2. Retrieval Results and Comparison with OMPS/LP

To evaluate the performance and quality of the retrieval scheme and results, the retrieved ozone profiles were compared with the OMPS/LP v2.6 ozone profile product provided by the NASA team [39], within spatial and temporal tolerances. For these two datasets, the latitude difference was restricted to within 1° , the longitude difference within 2° , and the satellite observation time difference to within 24 h. Figure 8 illustrates the orbital latitudes and longitudes measured by OMS-L and OMPS/LP on 1 August 2024, along with the corresponding observing points. Evidently, both instruments obtained matching points within corresponding tolerances across low, middle, and high latitude regions, with a relatively larger number of matching points in the northern high latitude.

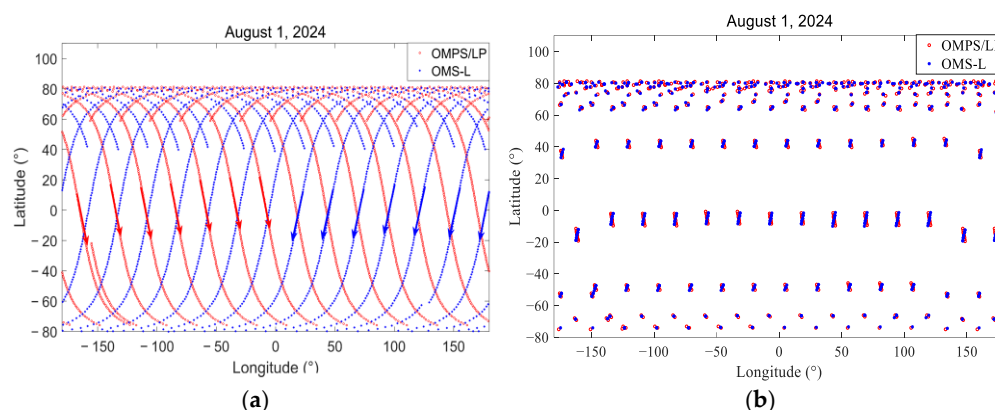


Figure 8. Observation points of OMS-L and OMPS/LP on the same day. (a) Latitudes and longitudes of all orbits. (b) Matched observation points.

The OMPS/LP v2.6 ozone profiles (hereinafter referred to as the product) provided by the NASA team were obtained through wavelength pairing and an optimal estimation algorithm with prior constraints [40]. The individual ozone profiles were retrieved by using combined UV and Vis measurements between 12.5 (or cloud top) and 57.5 km. For more details, refer to Table 3 and the Level 2 data release notes [39]. Retrieved surface albedo, cloud height, and TH correction were incorporated, and the aerosol extinction coefficients retrieved from OMPS/LP measurements were used in the forward model.

Table 3. Wavelengths used in the OMPS/LP v2.6 ozone retrieval, according to Kramarova et al. [39].

Parameters	Values
Wavelength used in UV (nm)	295, 302, 306, 312, 317, 322
Wavelength used in Vis (nm)	606
Reference wavelength used in UV (nm)	353
Reference wavelength used in Vis (nm)	510, 675
Normalization altitude used in UV (km)	60.5
Normalization altitude used in Vis (km)	40.5

3.2.1. Single Profile Comparison

To reduce the deviation in ozone profiles retrieval caused by a priori profile, in this subsection, the a priori profiles corresponding to specific latitudes are extracted from the OMPS/LP v2.6 dataset for single-profile retrieval. Figure 9 shows a comparison of nine single ozone profiles from OMPS/LP and OMS-L during the orbit at 00:47 on 1 August 2024. These results are highly representative, especially those selected at different latitudes, to demonstrate the similarity in the profile structures retrieved by the two instruments. As clearly shown in Figure 8, the retrieved ozone profiles closely follow the variations of the product. At different latitudes, both the peaks and shapes of the retrieved profiles

exhibit excellent agreement with those of the product profiles, indicating the feasibility and effectiveness of the retrieval scheme. Additionally, the retrieved profiles display good smoothness, particularly in low- and middle-latitude regions, suggesting the stability of the retrieval approach. However, at the beginning of the orbital scan (in the northern high-latitude region), the retrieved ozone profiles have lower peak values compared to the product. This phenomenon can be attributed to the large SZA at the start of the orbital scan, which approaches 90° . The weak solar radiance under such conditions leads to relatively large discrepancies in the retrieved ozone concentrations in high-latitude regions. Moreover, limb radiance is significantly influenced by the SZA. As the SZA decreases, the consistency between the retrieved ozone profiles and the product improves in low and mid latitudes.

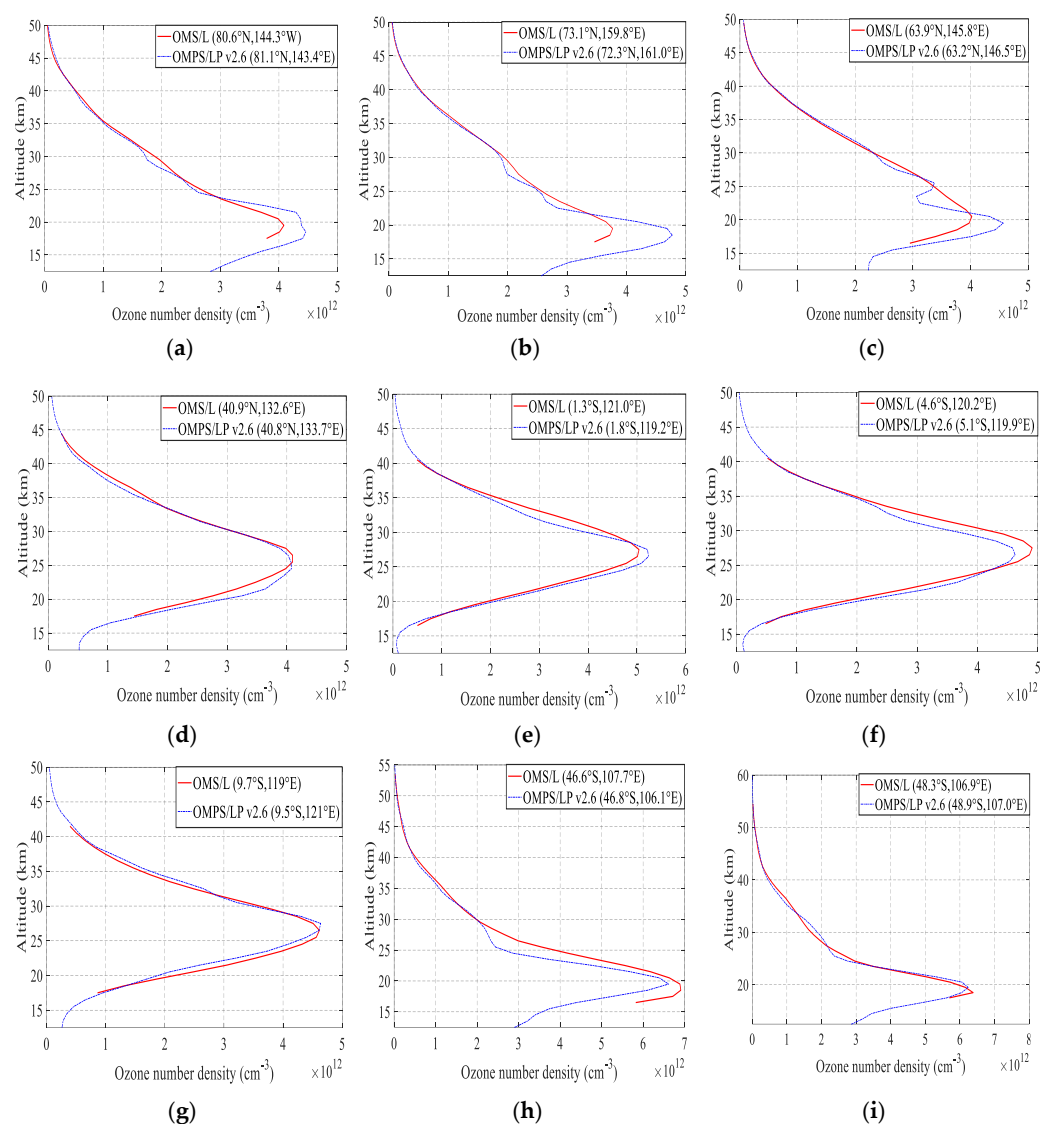


Figure 9. A selection of single profiles that meet the coincidence criteria at different latitudes, with a comparison between OMS-L and OMPS/LP v2.6. (a) OMS-L (80.6°N, 144.3°W) vs. OMPS-LP (81.1°N, 143.4°E); (b) OMS-L (73.1°N, 159.8°E) vs. OMPS-LP (72.3°N, 161.0°E); (c) OMS-L (63.9°N, 145.8°E) vs. OMPS-LP (63.2°N, 146.5°E); (d) OMS-L (40.9°N, 132.6°E) vs. OMPS-LP (40.8°N, 133.7°E); (e) OMS-L (1.3°S, 121.0°E) vs. OMPS-LP (1.8°S, 119.2°E); (f) OMS-L (4.6°S, 120.2°E) vs. OMPS-LP (5.1°S, 119.9°E); (g) OMS-L (9.7°S, 119°E) vs. OMPS-LP (9.5°S, 121°E); (h) OMS-L (46.6°S, 107.7°E) vs. OMPS-LP (46.8°S, 106.1°E); (i) OMS-L (48.3°S, 106.9°E) vs. OMPS-LP (48.9°S, 107.0°E).

3.2.2. Month Profiles Comparison

The processing results of the OMS-L L1 v1.2 data from August 2024 are presented, considering the observations when the SZA is less than 95° . It should be noted that the a priori profiles used for ozone profile retrieval in this section are from the built-in database of SCIATRAN. A total of 420 orbital datasets were processed, yielding approximately 50,000 profiles. Figure 10 shows a comparison between the retrieval results of OMS-L and the OMPS/LP v2.6 product, involving approximately 30,000 profiles in total. As clearly shown in Figure 10, the retrieved ozone concentrations between 12.5 and 45 km are higher than those of the product. At most altitudes, the relative difference is about 10%, with the maximum difference reaching about 30% at 15 km. The relatively large positive biases (10–15%) in the altitude range of 18–25 km are attributed to the fact that the retrieved ozone profiles in the high-latitude regions have larger peaks. One reason is that the retrieval wavelengths within this altitude range are associated with relatively strong limb stray light, and the other may be related to the large SZA at the start or end of the orbital scan.

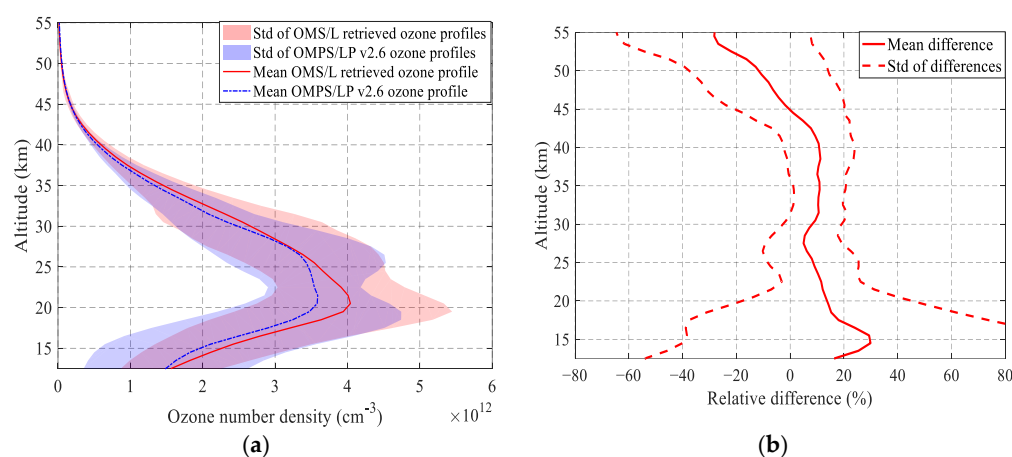


Figure 10. Comparison of the OMS-L retrievals and OMPS/LP v2.6. (a) Average profile (shaded areas are the standard deviation of the profile). (b) Mean relative difference (dashed line represents standard deviation of difference).

Since the minimum altitude at which OMS-L can retrieve ozone profiles is approximately 18 km, the ozone concentration in the region below 20 km is primarily determined by the a priori profiles. Consequently, this region demonstrates relatively large differences and low reliability. Above 45 km, the retrieved ozone concentration is lower than that of the product, and the negative bias increases with altitude. On the one hand, the relatively low ozone concentration in the upper stratosphere leads to significant retrieval deviations. On the other hand, the a priori profiles may be an important factor contributing to the retrieval deviations at the upper boundary.

Figure 11 illustrates a comparison between the OMS-L retrievals and OMPS/LP v2.6 profiles across six latitude bands. Below 20 km, large positive biases are observed in low-latitude regions, whereas negative differences are evident in high latitude areas. From 22 to 50 km, the differences remain within 10% for most altitudes, except at 40 km in the southern high latitude region and 45 km in the northern low latitude region, where the differences range from 15% to 20%. Above 45 km, the southern high latitude has positive biases in the range of 5–15%, while other latitudes show negative differences.

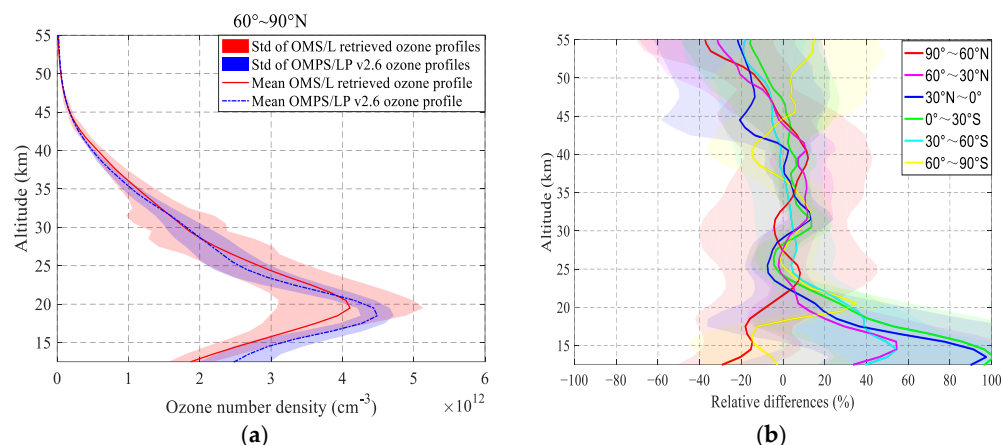


Figure 11. Comparison of the OMS-L retrievals and OMPS/LP v2.6. (a) Average profile in the northern polar region (shaded areas are the standard deviation of the profile). (b) Mean differences in six latitudinal bands (90°~60°N, 60°~30°N, 30°N~0°, 0°~30°S, 30°~60°S, 60°~90°S).

To provide a rigorous, quantitative assessment of the agreement, the comparisons were conducted using strict spatio-temporal coincidence criteria (latitude < 1°, longitude < 2°, time < 6 h). A comprehensive statistical analysis was performed, calculating the mean bias, standard deviation (SD, 1 σ), root-mean-square error (RMSE), and the number of collocated profiles (N) across different altitude and latitude bands. The complete results are presented in Supplementary Table S1 and Figure S4.

There is a relatively large positive bias (>50%) at the tropopause. This phenomenon can be attributed to multiple factors. Firstly, the ozone concentration at this altitude in low-latitude regions is extremely low, which accentuates the differences between the retrieved and reference values. Secondly, it is associated with the disparity in the lowest retrieval altitude of the two datasets. For OMS-L, the retrieval of ozone concentration below 20 km is largely governed by the a priori profile. Additionally, the retrieval differences caused by inaccuracies of surface albedo, aerosols, clouds, and atmospheric temperature and pressure reach their maximum values in this altitude range. Furthermore, OMS-L conducts retrieval in the 332 nm UV band. According to the weighting function, the sensitivity of this wavelength to ozone changes is substantially reduced, while the OMPS/LP v2.6 product employs the triplet method retrieval in the visible band. The differences in the retrieved results between OMS-L and the product can be ascribed to various factors, including specific retrieval settings such as the ozone absorption cross-section, a priori profile, surface albedo, and aerosol parameters. Moreover, disparities in retrieval spectra and algorithms also contribute to these differences. Despite these variations, the OMS-L retrieval results demonstrate relatively good agreement with the OMPS/LP v2.6 product, particularly in the upper-middle stratosphere.

4. Discussion

This study successfully demonstrates the capability of FY-3F/OMS-L to retrieve stratospheric ozone profiles with high vertical resolution. The retrieval scheme, based on UV wavelength pairing and WMART, proves effective for altitudes of 18–55 km.

The weighting factors in the WMART algorithm were applied uniformly in this global retrieval. The value of $\mathbf{W}^{\text{LOS}}$ is determined by the fixed limb-viewing geometry and is thus invariant. Although the radiance and retrieval vectors exhibit latitudinal and seasonal variations, the sensitivity of the final retrieved profile to the specific values of $\mathbf{W}^{\text{pair}}$ is low, as noted by Degenstein et al. [29]. Our experiments align with this finding, showing that the crucial function of $\mathbf{W}^{\text{pair}}$ is to enforce a smooth and monotonic transition of information

between altitude layers. Consequently, a single, well-tuned set of W^{pair} values is sufficient for generating stable and physically plausible ozone profiles on a global scale, without the need for geographical or seasonal tuning.

The sensitivity analysis confirms that tangent height accuracy is the most critical factor, underscoring the importance of precise geometric calibration. Other parameters like a priori profile and ozone cross-section temperature also contribute significantly to the total error budget. The total error estimation assumes independence among error sources, a common simplification for initial retrievals; future work should incorporate error covariance modeling for a more rigorous uncertainty assessment.

The retrieved ozone profiles show generally good agreement with the OMPS/LP v2.6 dataset, notably within the 22–50 km altitude range, where the differences are consistently within 10%. The discrepancies observed at the profile boundaries (below 20 km and above 45 km) are understandable and common in profile retrievals. The methodological differences between OMS-L and OMPS/LP contribute to the observed systematic offsets. Key differences include: (1) Wavelength selection: OMS-L uses only UV wavelengths, while OMPS/LP combines UV and visible bands, giving it better sensitivity in the lower stratosphere and troposphere. This is a primary reason for the larger biases below 20 km. (2) A priori information: The two retrievals use different a priori profiles and constraints. (3) Aerosol treatment: OMPS/LP retrieves aerosol extinction, whereas OMS-L uses a fixed background climatology, which can lead to biases under elevated aerosol conditions. (4) Cloud screening and surface albedo: Our retrieval employed a fixed surface albedo and did not correct for the presence of clouds. In contrast, the OMPS/LP product incorporates cloud screening and a more dynamic surface albedo correction. This key difference likely explains a significant portion of the positive bias observed in OMS-L retrievals in the lower atmosphere, particularly near the tropopause.

5. Conclusions

The limb spectra measured by OMS-L in the Hartley–Huggins band were used to retrieve the ozone profiles from 18 to 55 km based on wavelength pairing and the WMART algorithm. The retrieved ozone profiles were compared with the OMPS/LP v2.6 ozone profiles provided by the NASA team. The results demonstrated that the OMS-L retrievals were generally in good agreement with the product, with a deviation of less than 10% in the range of 22–50 km. There is an overall good agreement between the retrieved results and the product at all latitude bands, with differences typically within $\pm 10\%$, except at 40 km in the high-southern latitude and 45 km in the low-northern latitude. Although larger differences were observed below 20 km, on the one hand, this could be ascribed to the difference in the lowest retrieval altitude of the two datasets. On the other hand, it was likely associated with the small ozone amount, large dynamic changes in this region, and the reduced sensitivity of ozone detection resulting from the UV retrieval wavelengths employed by OMS-L. As a consequence, there was a large uncertainty in the OMS-L ozone concentration retrieval in this region. Error analysis of the minimum offset revealed that the overall estimated error for ozone profile retrieval was 5–30%. Besides the recognized largest error source of incorrect TH registration, additional error sources were the uncertainties of the a priori ozone profile and the temperature-dependent cross-section. Despite the differences in retrieval parameter settings and algorithms between OMS-L and the reference product, the resulting deviations remained within an acceptable range.

OMS-L is the first UV-Vis hyperspectral atmospheric limb-sounding payload in China. The ozone profiles were retrieved from OMS-L UV measurements in the upper-middle stratosphere for the first time. The findings of this research indicate that OMS-L can measure stratospheric ozone profiles with high vertical resolution, providing high quality

stratospheric ozone profile data support for related fields such as stratospheric atmospheric chemistry research and climate change assessment, and contributing to enhancing China's influence and leading role in the global arena of stratospheric ozone monitoring and research.

Supplementary Materials: The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/rs17233784/s1>, Figure S1: Representative examples of observed and modeled Hartley Pairing Vectors (HPVs) and residuals. Figure S2: The effect of changing the number of retrieval iterations performed by the SCIATRAN model on the final ozone profile. Figure S3: Averaging kernels of the OMS-L ozone profile retrieval. Figure S4: Comparison of the OMS-L retrievals and OMPS/LP v2.6 under a stricter temporal window. Table S1: Statistical comparison of OMS-L and OMPS/LP v2.6 ozone profiles.

Author Contributions: Conceptualization, F.Z. and S.L.; methodology, F.Z.; software, F.Z.; validation, F.Z., S.L. and F.S.; formal analysis, F.S.; investigation, F.Z.; resources, F.Z.; data curation, F.Z.; writing—original draft preparation, F.Z.; writing—review and editing, F.Z.; project administration, S.L.; funding acquisition, S.L. All authors have read and agreed to the published version of the manuscript.

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Data Availability Statement: The OMS-L L1 V1.2 data from August 2024 used for ozone profile retrieval in this study can be ordered from the website: <https://satellite.nsmc.org.cn/DataPortal/cn/home/index.html>, last access: 20 September 2024. The OMPS/LP v2.6 ozone profile product used for validation is available at https://disc.gsfc.nasa.gov/datasets/OMPS_NPP_LP_L2_O3_DAILY_2.6/, last access: 2 October 2024. Sample OMS-L L2 data and the retrieval code used in this study are available from the corresponding author upon reasonable request.

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