



Article Retrieval of Stratospheric Ozone Profiles from Limb Scattering Measurements of the Backward Limb Spectrometer on Chinese Space Laboratory Tiangong-2: Preliminary Results

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Abstract: The Backward Limb Spectrometer (BLS) onboard the Tiangong-2 (TG-2) space laboratory, the first spaceborne limb sounding instrument of China, was successfully launched on 15 September 2016, and its measurements of scattered photons of sunlight along the limb line-of-sight (LOS) in the 290–1000 nm range could be used to derive the vertical distribution of stratospheric ozone with high vertical resolution. Ozone profiles with a vertical resolution of one km in 10–40 km and 30–50 km were retrieved by the triplet and pair methods, respectively, and the ozone profiles retrieved by the BLS were compared with the ozone sounding data over four sounding stations. Meanwhile, the Ozone Mapping and Profiler Suite Limb Profiler (OMPS/LP) version 2.5 (v2.5) stratospheric ozone profile product was also introduced for comparison. The retrieval results showed a good agreement with the ozone profiles of ozone sounding and the OMPS/LP v2.5 product, and the differences were basically within 25% above 20 km, while relatively larger differences occasionally occurred below 20 km. The case studies over four sites worldwide demonstrate that the BLS is capable of measuring stratospheric ozone profiles with high vertical resolution.

Keywords: ozone profile; limb sounding; Tiangong-2; OMPS/LP

1. Introduction

As an essential component of the Earth's atmosphere, stratospheric ozone not only protects life by absorbing short-wave ultraviolet (UV) radiation but also plays a vital role as an energy influencer and oxidant in atmospheric circulation and chemical processes [1–3]. Since the 1980s, a series of ozone layer protection policies have been proposed due to the discovery of the Antarctic ozone hole [4]. There is ample evidence that these policies have yielded remarkable results, and the stratospheric ozone is recovering [5–8]. Nevertheless, large areas of abnormally low ozone concentrations have been detected over the Arctic in the winter and spring of recent years, and the physical and chemical processes behind the above phenomena require a deeper understanding [9–11]. Furthermore, the material exchange between the troposphere and the stratosphere involving stratospheric ozone has also been a hot issue in recent years. Pollutants from the troposphere can enter the stratosphere through deep convection, leading to the depletion of stratospheric ozone [12], and stratospheric ozone can also enter the troposphere to cause tropospheric ozone pollution, resulting in the so-called stratospheric ozone intrusion [13]. Finer ozone profile observations with high vertical resolution are necessary for the study of the above problems.

Currently, ozone profiles are generally measured through ozonesonde carried by balloon or spectral radiation from ground-based or satellite observations. The ozonesonde measurements are often used as standard reference but only a handful of weekly records



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Copyright: © 2022 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). are available globally [14,15]. Ground-based measurements by Brewer or Dobson could provide ozone profiles during sunrise and sunset through the Umkehr method under a cloudless sky, but these observations are sparsely and non-uniformly distributed in the world [16,17]. However, satellite observations, either nadir- or limb-viewing, can provide global coverage and long-term ozone profile observations. The nadir-viewing is the most popular method for spaceborne instruments, such as the second generation of Solar Backscattered UltraViolet (SBUV/2) instrument, the Global Ozone Monitoring Experiment (GOME) instrument and the Ozone Monitoring Instrument (OMI), but it is more suitable for obtaining total ozone than profiles due to its relatively lower vertical resolution [18–24]. The limb observation, or its special mode occultation that looks directly at the sun, can be used to derive ozone profiles with high vertical resolution through slicing the atmosphere into several thinner layers [25,26]. It has been successfully applied by the Scanning Imaging Absorption Spectrometer for Atmospheric Cartography (SCIAMACHY), the Optical Spectrograph and Infrared Imager System (OSIRIS), the Ozone Mapper and Profile Suite Limb Profiler (OMPS/LP) and the Stratospheric Aerosol and Gas Experiment (SAGE) family series [27–31].

On 15 September 2016, China launched its first limb sounding instrument, the Backward Limb Spectrometer (BLS), which was mounted on the Tiangong-2 (TG-2) space laboratory and was supposed to provide vertical profiles of ozone in the stratosphere with high vertical resolution. In this paper, an algorithm for retrieving ozone profiles between 10 and 50 km from limb scattering radiance (LSR) data obtained by BLS was developed, and the triplet and pair methods were introduced in the algorithm to derive the ozone profiles within 10–40 km and 30–50 km, respectively. The retrieval results of the BLS are compared with ozone sounding data and OMPS/LP version 2.5 (v2.5) stratospheric ozone profile product over four sites where ozone-sounding data is available.

2. Materials and Methods

2.1. Materials

2.1.1. The BLS on TG-2

Among the payloads on the second generation of the Chinese space laboratory TG-2, the BLS (as shown in Figure 1a) is the first Chinese spaceborne instrument with limb sounding abilities. It worked in space for almost three years, until July 2019, due to the scheduled termination of the TG-2 service. The BLS is a spectrometer that utilizes a prism as the dispersive element (as shown in Figure 1b), which covers the spectrum from 290 to 1000 nm with a varied resolution from 1.2 (@290 nm) to 22.4 nm (@1000 nm) [32]. An enhanced UV-coated CCD was used by the BLS to improve the signal-to-noise ratio (SNR) in the UV band. The design intention and principle of the BLS are similar to OMPS/LP, and several of their main performance parameters are listed in Table 1 for comparison [33–35].

The line-of-sight (LOS) of the BLS points in the opposite direction to the movement of TG-2 (as shown in Figure 1c), which is the origin of term "Backward" in its name. The LOS of the BLS is also tangent to the atmosphere (as shown in Figure 1d), and the measurements of scattered photons of sunlight along the LOS at different tangent heights (THs) can be used to extract ozone profiles.

Table 1. Several main performance parameters of BLS and OMPS/LP.

Item	BLS	OMPS/LP
Spectral coverage	290–1000 nm	290–1000 nm
Spectral resolution	1.2–22.4 nm	1.5–30 nm
Vertical coverage	10–60 km	Tropopause–60 km
Vertical resolution	~3 km	~1 km



Figure 1. Some information about the BLS, including: (**a**) appearance; (**b**) optical layout; (**c**) a schematic diagram of the field of view (orange shadow), and the white arrow indicates the flight direction of TG-2; (**d**) viewing geometry. (**a**,**b**) are from Li et al., (2019) [36].

2.1.2. The BLS Level-1B Version 1.02 LSR Data

The BLS Level-1B version 1.02 (L1B v1.02) LSR data used for ozone profile inversion in this paper is the product of geographical registration and spectral and stray light correction.

Unlike polar orbital satellites, the orbital inclination of TG-2 is about 42°, so BLS observations are mainly focused between 43°N and 43°E (as shown in Figure 2a). The overpassing time of TG-2 is about 10:30 a.m. (local time). Limited by the overall mission commands and power supply of TG-2, the BLS could only work for a maximum of about 20 min per orbital cycle, which resulted in the irregular spatial-temporal distribution of BLS observations. The upper panel in Figure 2 shows the orbits where BLS observations were available on 22 September 2016, and the lower panel plots a set of sample spectra measured by BLS at different THs over 40.50°N and 29.38°E on the same day. The ozone absorption bands, such as at 600 nm, can be seen in Figure 2b, which are the basis for extracting ozone profiles from the LSR data.





2.1.3. A Priori Data

The sources of a priori data used in this paper are listed in Table 2. The temperature and pressure profiles used in retrieval are all from the MERRA-2 reanalysis data, which can provide profiles from 985 hPa to 0.01 hPa with a horizontal resolution of $0.5^{\circ} \times 0.625^{\circ}$ and a temporal resolution of 3 h [37]. Profiles of ozone and other absorbing gases (e.g., nitrogen dioxide, etc.) were obtained from a built-in database in SCIATRAN (detailed in Section 2.1.5), which was output from a 2D chemical transport model, including a variety of gases with significant absorption in the UV-vis-IR band [38]. This database divides the global into 18 latitude zones at 10° intervals, and each zone contains 12 monthly average data sets with an altitude range from 1 to 95 km. Aerosol parameters are set according to LOWTRAN aerosol parameterization in SCIATRAN [39]. The surface albedo data comes from the Matthews database, a global dataset with a horizontal resolution of $1^{\circ} \times 1^{\circ}$, based on a variety of data and satellite images [40].

Table 2. The sources of a priori data used in retrieval.

Sources		
MERRA-2 reanalysis data		
MERRA-2 reanalysis data		
A database embedded in the SCIATRAN		
A database embedded in the SCIATRAN		
LOWTRAN aerosol parameterization		
Matthews global database		

2.1.4. Data for Accuracy Verification

To verify the accuracy of retrieval results, ozone profiles obtained from four ozone sounding stations (i.e., Beijing, Boulder, Hilo, and Hong Kong) that overlap in space and time with BLS observations were introduced. The ozone sounding data is obtained by electrochemical concentration cell (ECC) ozonesonde carried by a balloon, which can generally provide ozone profiles from the surface to an altitude of about 35 km. It has been evaluated with high accuracy and can be used as a benchmark for comparison [41]. Meanwhile, the ozone profiles from the OMPS/LP v2.5 stratospheric ozone profile product closest in space and time with the four ozone sounding stations were also introduced for comparison. The ozone profiles in the OMPS/LP v2.5 product were processed into a regular grid with a vertical resolution of 1 km, including upper and lower parts. The upper part (~30 to ~50 km) is retrieved from the ultraviolet bands, and the lower part (tropopause to ~37 km) is retrieved from the visible bands [35].

2.1.5. Forward Model

In limb sounding, the light path in the atmosphere is very long (as shown in Figure 1d), so the forward modeling of limb radiances must be performed under a spherical atmosphere to account for the curvature of the Earth. The SCIATRAN version 3.8.13 (v3.8.13) was selected as the forward model in this study, which has a spectral range of 0.18–40 μ m and can provide plane-parallel, pseudo-spherical, and spherical atmospheric modes [42,43].

For ozone profile inversion, in this study, a horizontal homogeneous spherical grid with a vertical resolution of 1 km was used in SCIATRAN, so the vertical resolution of the retrieved ozone profiles was also 1 km. To trade off computation cost and accuracy, the single scattering was performed in fully spherical geometry, while the multiple scattering contribution was approximated in a pseudo-spherical atmosphere.

2.2. Methods

2.2.1. TH Registration

Almost all atmospheric components and elements vary significantly with height, therefore the accuracy of TH is crucial for extracting ozone profiles from the LSR data. As shown in Figure 1d, the distance between the instrument and the tangent point (TP) is very far, and a minor pointing error of the LOS may lead to a large deviation in the TH due to the magnification of this distance. The distance between the BLS and the TP is generally greater than 2000 km, and a pointing error of 0.01° will result in an error of about 400 m in TH. The TH values given in the BLS L1B v1.02 data were preliminary results derived from orbital geometry, spacecraft attitude, etc., and their inaccuracy made it hard to meet the requirements of subsequent ozone profile inversion. Consequently, TH registration must be done before ozone profile inversion.

Several approaches have been proposed to correct TH, among them the three most commonly used are the Rayleigh scattering attitude sensing (RSAS) method, the knee method, and the absolute radiance residual method (ARRM) [44–46]. In this study, the ARRM was used to perform TH registration on the BLS L1B v1.02 data. In ARRM, two quantities are first defined, the residual $r(\lambda, H)$ and the slope $s(\lambda, H)$, which are written as:

$$\mathbf{r}(\lambda, H) = \ln I_m(\lambda, H) - \ln I_s(\lambda, H) \tag{1}$$

$$s(\lambda, H) = \partial ln I_s(\lambda, H) / \partial H$$
⁽²⁾

where $I_m(\lambda, H)$ and $I_s(\lambda, H)$ are the measured and simulated radiances at wavelength λ and TH H, respectively. And then, the TH corrected value Δz can be given by:

$$\Delta z = \left\{ \mathbf{r}(\lambda, H) - \left[\mathbf{r}(\lambda_a, H) - \mathbf{r}(\lambda_a, H_0) \right] \right\} / \left\{ \mathbf{s}(\lambda, H) - \left[\mathbf{s}(\lambda_a, H) - \mathbf{s}(\lambda_a, H_0) \right] \right\}$$
(3)

where λ and λ_a are set to 295 nm and 350 nm, respectively; *H* and *H*₀ are set to 65 km and 40 km, respectively. The theoretical basis and detailed description of the ARRM can be found in the paper published by Moy et al. in 2017, which will not be repeated here [46]. The ARRM had been applied to the OMPS/LP v2.5 stratospheric ozone profile product [35].

2.2.2. Retrieval Vector

The algorithm for retrieving ozone profiles from BLS LSR data is based on the fact that the LSR at certain wavelengths is highly sensitive to changes in ozone concentration, and the partial derivative of the logarithm of LSR to the logarithm of ozone concentration can be used as a sensitivity parameter, which is known as a weighting function, kernel function, or Jacobian matrix:

$$w(\lambda, H, h) = \partial ln I(\lambda, H) / \partial ln N_{O3}(h)$$
(4)

where $w(\lambda, H, h)$ is the weighting function, $I(\lambda, H)$ is the LSR of the wavelength λ at the TH *H*, and $N_{O3}(h)$ is the ozone number density at the height *h*. In those bands where ozone has strong absorption, the weighting function peaks when *H* is equal to *h*. This is caused by the longest path of the LOS in the level tangent to it in limb-viewing geometry. Figure 3

shows the peak sensitivity of the LSR from 280 to 1000 nm to the ozone number density at different altitudes calculated by SCIATRAN under a given viewing condition. In the UV band, photons can penetrate to a lower altitude with the increase of wavelength due to the weakening of its absorption by ozone (as shown by the deep pink solid line in Figure 3), but it is generally only sensitive to ozone above 20 km. Compared with UV light, visible light around 600 nm is relatively weakly absorbed by ozone, which can be used to detect ozone down to about 10 km. Therefore, it is only possible to retrieve the entire stratospheric ozone profiles from the LSR data by combining UV and visible bands. The 320 nm and 600 nm bands were used in this paper to retrieve upper (30–50 km) and lower (10–40 km) ozone profiles, respectively.



Figure 3. The peak sensitivity of the LSR I from 280 to 1000 nm to the ozone number density N_{O3} at different altitudes calculated by SCIATRAN under a given viewing condition (solar zenith angle of 45°; relative azimuth angle of 45°, i.e., the angle of the LOS relative to the sun). The blue solid line is the corresponding ozone profile. The deep pink solid line is the absorption cross-section of ozone at 273 K.

In the practical process of extracting ozone profiles from LSR data, there are still many uncertainties, such as surface albedo, clouds, and Rayleigh scattering and stratospheric aerosols. This means that the retrieval of ozone profiles cannot be realized by directly establishing the relationship between the LSR and ozone concentration, but by constructing a retrieval vector to remove or reduce the interferences cause by the above uncertainties [47]. As a whole, the construction of the retrieval vector includes two steps. The first step is radiance normalization, which can be written as:

$$I_n(\lambda, H) = I(\lambda, H) / I\left(\lambda, H_{ref}\right)$$
(5)

where $I_n(\lambda, H)$ is the normalized radiance; H_{ref} is reference TH, which is generally greater than 40 km to avoid the influence of stratospheric aerosols, but it should not be too high to weaken the noise contamination. Here we set H_{ref} equal to 45 km and 55 km for the retrieval of ozone profiles within 10–40 km and 30–50 km, respectively. The radiance normalization can effectively reduce the influence of surface albedo, clouds, and even absolute calibration error. In the second step, the retrieval of the upper ozone is different from that of the lower ozone. For the ozone profiles between 30 and 50 km, the normalized radiances at a wavelength λ_s , strongly absorbed by ozone, and a wavelength λ_w , weakly absorbed by ozone, are used to construct the retrieval vector y_{pair} , and its element $y_{pair}(H)$ can be written as:

$$y_{vair}(H) = \ln[I_n(\lambda_s, H) / I_n(\lambda_w, H)]$$
(6)

We named it the pair method, as indicated by the subscript "pair". Here we set λ_s and λ_w to be 320 nm and 355 nm, respectively.

For the ozone profiles between 10 and 40 km, the retrieval vector y_{tri} is composed of normalized radiances at a wavelength λ_0 , strongly absorbed by ozone, and two wavelengths at λ_1 and λ_2 , which are relatively weakly absorbed by ozone, and its elements $y_{tri}(H)$ can be written as:

$$y_{tri}(H) = \ln \left[I_n(\lambda_0, H) / \sqrt{I_n(\lambda_1, H)I_n(\lambda_2, H)} \right]$$
(7)

Here we set λ_0 , λ_1 , and λ_2 to be 600 nm, 525 nm, and 675 nm, respectively. This method is named the triplet method. The retrieval vectors constructed by the pair method and the triplet method can effectively reduce the impact of inaccurate estimation of Rayleigh scattering and stratospheric aerosols on the retrieval results.

2.2.3. Optimal Estimation Method

An optimal estimation method for minimizing the cost function was used in the ozone profile inversion in this paper, and the ozone profiles were derived through the Gauss–Newton iteration [48]. The iterative formula is:

$$\boldsymbol{x}_{i+1} = \boldsymbol{x}_a + \left(\boldsymbol{K}_i^T \boldsymbol{S}_{\varepsilon}^{-1} \boldsymbol{K}_i + \boldsymbol{S}_a^{-1}\right)^{-1} \boldsymbol{K}_i^T \boldsymbol{S}_{\varepsilon}^{-1} [\boldsymbol{y} - \boldsymbol{F}(\boldsymbol{x}_i) + \boldsymbol{K}_i (\boldsymbol{x}_i - \boldsymbol{x}_a)]$$
(8)

where x_a is the a priori ozone profile, and x_a in each iteration is replaced by the x_i calculated in the previous iteration, which can reduce the dependence on the a priori ozone profile; x_i and x_{i+1} are the ozone profiles derived from the *i*th iteration and the (i + 1)th iteration, respectively; y is the measured retrieval vector; $F(x_i)$ is the simulated retrieval vector obtained through SCIATRAN; K_i is the weighting function simulated by SCIATRAN at x_i ; and S_a and S_e are the covariance matrices of the a priori ozone profile and measurement noise, respectively. The final retrieval results can be derived through the iteration of Equation (8).

3. Results

3.1. Sensitivity Analysis

The theoretical accuracy of the retrieval results can be roughly estimated by sensitivity analysis. Several main parameters that affect retrieval accuracy are discussed below.

3.1.1. Pointing Error

As mentioned in Section 2.2.1, the accuracy of TH is critical for extracting ozone profiles from the LSR data. The sensitivity of the retrieval results to the pointing error is simulated by artificially shifting the LSR data up or down by an offset. Figure 4 shows the changes in the retrieved upper and lower ozone profiles when the LSR data are shifted upward or downward by 0.5 km and 1.0 km. An offset of 1.0 km for TH will result in a maximum error of about 25% in the ozone profiles.

Although the ARRM had been used for TH registration in this paper, it is difficult to guarantee the absolute accuracy of TH. The primary reason for this is that the LSR measurements at 295 nm are used in the ARRM, which makes the TH correction very sensitive to instrument calibration. Figure 5 shows the sensitivity of the TH correction to the LSR at 295 nm. If the LSR at 295 nm is artificially increased or decreased by 1%, there



will be an error of about 100 m in the correction value of TH. Moreover, the ARRM is also affected by stratospheric aerosols [46].

Figure 4. (**a**,**c**) are the retrieved upper and lower ozone profiles when the LSR data are shifted by different heights, respectively. (**b**,**d**) are the differences between the ozone profiles in (**a**,**c**) and the corresponding assumed true ozone profiles, respectively. The black solid lines in (**a**,**c**) represent the "true" ozone profiles. The red dashed lines and solid lines represent shifting of the LSR data upward by 0.5 km and 1.0 km, respectively. The blue dashed lines and solid lines represent shifting of the LSR data downward by 0.5 km and 1.0 km, respectively.



Figure 5. Sensitivity of the TH correction values obtained by the ARRM to the LSR at 295 nm. The black solid line represents the deviations of the TH that still exist after the ARRM registration when different perturbations are artificially added to the TH. The red solid and dashed lines are the TH deviation curves after artificially increasing and decreasing the LSR at 295 nm by 1%, respectively.

3.1.2. Surface Albedo and Clouds

The imperfect estimation of surface albedo and clouds in forward modeling will directly affect the retrieval accuracy. Though the effects of surface albedo and clouds are assumed to be eliminated by radiance normalization in the current algorithm, they cannot be completely eliminated, in practice. The sensitivity of the retrieved ozone profiles to surface albedo was simulated and analyzed, and the results are shown in Figure 6. The surface albedo mainly affected the retrieval of the lower ozone profiles, while its effects on the upper ozone profiles could be ignored. Even for the retrieval of lower ozone profiles, its effects were not significant due to the radiance normalization. The maximum error can be more than 10% when the surface albedo is 0.7. However, the extreme cases of such a large deviation from the true albedo in the retrieval are very rare, in practice. As mentioned in Section 2.1.3, the Matthews global albedo database used in retrieval also avoids such extreme cases to the greatest extent.



Figure 6. (**a**,**c**) are the upper and lower ozone profiles retrieved under different surface albedo conditions, respectively. Different colors represent different surface albedos, and the true surface albedo is assumed to be 0.2. (**b**,**d**) are the differences between the ozone profiles in (**a**,**c**) and the corresponding assumed true ozone profiles, respectively.

Clouds are not considered in this paper. To analyze the influence of clouds on the retrievals, a layer of water clouds with an optical thickness of 20 (@500 nm) between 2.5 km and 3.0 km was added in simulation, but a cloudless sky is assumed in the retrieval, and the results are given in Figure 7. Similar to surface albedo, clouds also mainly affect the retrieval of lower ozone profiles, with negligible effects on upper ozone profiles. However, the influence of clouds is greater than that of the surface albedo, and the differences can exceed 20% at 10 km.



Figure 7. (**a**,**c**) are the upper and lower ozone profiles retrieved under cloudy (black solid lines) and cloudless (red solid lines) conditions, respectively. (**b**,**d**) are the differences between the ozone profiles retrieved under cloudless and cloudy conditions in (**a**,**c**), respectively.

3.1.3. Stratospheric Aerosols

Stratospheric aerosols are mainly sulfuric acid droplets with a concentration of 75%, which generally originate from volcanic eruptions and exist below 40 km. Figure 8 presents the stratospheric aerosol extinction coefficient profiles at 550 nm for the background and moderate volcanic periods assumed in SCIATRAN. We assume there exists a moderate volcanic event in the stratosphere, but the background stratospheric aerosol loading is used in the retrieval, and the results are presented in Figure 9. Stratospheric aerosols mainly affect the retrieval of the lower ozone profiles, and the error due to the imperfect estimation of stratospheric aerosols may exceed 20%. In the absence of large volcanic eruptions, the loading of stratospheric aerosols is relatively low and stable, and the direct use of background stratospheric aerosol loading will not have a great impact on the retrieval of the lower ozone profiles.



Figure 8. Stratospheric aerosol extinction coefficient profiles at 550 nm during background and moderate volcanic periods.



Figure 9. (**a**,**c**) are the upper and lower ozone profiles retrieved under different loading of stratospheric aerosols, respectively. The black and red solid lines represent moderate volcanic and background conditions, respectively. (**b**,**d**) are the differences between the ozone profiles retrieved under background and moderate volcanic conditions in (**a**,**c**), respectively.

3.2. Retrieval Results and Comparison

To verify the accuracy of the retrieval results, four rectangular zones ranging $\pm 5^{\circ}$ longitude and $\pm 3^{\circ}$ latitude were delineated around the four ozone sounding stations mentioned in Section 2.1.4. The ozone profiles were retrieved from BLS observations that fell within the above four zones and were closest to the corresponding ozone sounding stations, and the BLS observation time was required to be within 24 h before or after the ozone sounding acquisition time. Moreover, the ozone profiles from OMPS/LP v2.5 product closest in space and time to the ozone sounding were also introduced for comparison. The details involved in the above are listed in Table 3.

The ozone profiles retrieved from BLS and derived from ozone sounding and OMPS/LP v2.5 product are given in Figure 10, and the differences among them are given in Figure 11. In Figure 11, since the vertical resolution of ozone profiles obtained by ozone sounding and the BLS was different, the vertical resolution of ozone sounding was adjusted to be consistent with the BLS by simple linear interpolation. The ozone profiles from the BLS agree with those of ozone sounding and OMPS/LP very well above 20 km. Compared with the OMPS/LP product, the differences in ozone profiles retrieved from the BLS by the pair method are basically within 25% above 40 km (as shown in Figure 11), and larger differences occasionally occur below 40 km. According to the sensitivity analysis above, this situation is mainly caused by the pointing error. For the upper ozone profiles, the gradient of ozone concentration in the vertical direction above 40 km is relatively small, while the ozone concentration increases rapidly with the decrease of altitude below 40 km. Compared with the ozone sounding data, the differences of ozone profiles retrieved from the BLS by the BLS by the triplet method were basically within 25% above 20 km, and the larger

differences often appeared below 20 km. The larger differences below 20 km were mainly caused by the pointing error and clouds. Ozone concentration below 20 km is relatively low, and the absolute error of ozone number density caused by the larger percentage difference was not that large.



Figure 10. Ozone profiles obtained from the BLS, ozone sounding, and OMPS/LP at different times over the four ozone sounding stations in Beijing (**a**,**b**), Boulder (**c**), Hilo (**d**), Hong Kong (**e**–**g**). The red solid and dashed lines represent the lower and upper ozone profiles retrieved from the BLS, respectively; the green solid and dashed lines represent the lower and upper ozone profiles extracted from the OMPS/LP v2.5 product, respectively; the blue solid lines are ozone profiles obtained by ozone sounding.



Figure 11. The differences between the retrieval results and the corresponding benchmarks in Beijing (**a**,**b**), Boulder (**c**), Hilo (**d**), Hong Kong (**e**–**g**). (**h**) is the legend. The red and green solid lines represent the differences between the lower ozone profiles derived from the BLS and OMPS/LP v2.5 product and the ozone sounding data, respectively. The red dashed lines indicate the differences between the upper ozone profiles of the BLS and OMPS/LP v2.5 product.

Ozone Sounding			BLS		OMPS/LP	
Station	Location	Acquisition Time	Location	Acquisition Time	Location	Acquisition Time
Beijing	39.81°N, 116.47°E	27 September 2016 05:59	39.06°N, 117.02°E	27 September 2016 01:21	36.78°N, 105.09°E	27 September 2016 05:59
		16 January 2018 05:52	38.42°N, 115.37°E	15 January 2018 07:17	37.82°N, 111.01°E	16 January 2018 05:33
Boulder	39.95°N, 105.20°W	4 January 2017 19:36	38.36°N, 103.77°W	4 January 2017 17:52	38.23°N, 109.62°W	4 January 2017 20:15
Hilo	19.72°N, 155.05°W	4 January 2017 18:59	17.28°N, 151.40°W	4 January 2017 19:18	19.76°N, 155.29°W	4 January 2017 23:33
Hong Kong 22. 114		16 August 2017 05:21	23.19°N, 114.15°E	15 August 2017 05:16	24.89°N, 122.71°E	16 August 2017 04:58
	22.31°N, 114.17°E	4 October 2017 05:27	19.88°N, 110.77°E	3 October 2017 08:50	19.85°N, 103.28°E	4 October 2017 06:19
		7 March 2018 05:23	25.34°N, 119.36°E	6 March 2018 08:41	24.73°N, 124.34°E	7 March 2018 04:51

Table 3. The locations and acquisition times of the four ozone sounding stations and their corresponding closest BLS and OMPS/LP.

4. Discussion

Based on the sensitivity analysis in Section 3.1, the retrieval of upper ozone profiles was mainly affected by the pointing error, while the retrieval of lower ozone profiles was not only affected by the pointing errors but also by clouds. In the current version of the algorithm, only a cloudless sky was assumed. A more complicated and "real" atmosphere including clouds should be considered in future versions. Besides, the TH information in the BLS LSR data was corrected through the ARRM, but the ARRM is vulnerable to calibration error and stratospheric aerosols. A more general and stable TH registration method is also the focus of future work.

5. Conclusions

In this paper, an algorithm for retrieving ozone profiles from 10 to 50 km was developed for the first Chinese space limb sounding instrument, the BLS. The ARRM was used to perform TH registration, and then the triplet and pair methods were adopted for retrieving the ozone profiles within 10–40 km and 30–50 km zones, respectively. The preliminary retrieval results show that the ozone profiles retrieved from the BLS were in good agreement with those of ozone sounding and OMPS/LP, and the differences were basically within 25% above 20 km. The larger errors were prone to occur below 20 km, which were mainly caused by pointing errors and clouds.

Unlike operational instruments, the BLS is only a preliminary instrument for limb sounding and coupled with the power constraints of space laboratory, the amount of ozone sounding data available for verification is very limited. The results of several case studies in this research demonstrate that the BLS is capable of measuring stratospheric ozone profiles with high vertical resolution.

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Data Availability Statement: The BLS L1B V1.02 LSR data used for ozone profile inversion in this paper can be ordered from the website: http://www.msadc.cn/main/product, accessed on

11 May 2021. The MERRA-2 reanalysis data used in this paper is available at https://disc.gsfc. nasa.gov/datasets?project=MERRA-2, accessed on 21 August 2021. The sources of ozone sounding data used for verification include the Global Monitoring Laboratory (GML) of NOAA (available at https://gml.noaa.gov/aftp/data/ozwv/Ozonesonde/, accessed on 26 March 2021), which provides data of the Boulder and Hilo stations, the World Ozone and Ultraviolet Radiation Data Centre (WOUDC) (available at https://woudc.org/data/explore.php, accessed on 4 August 2021), which provides data of the Hong Kong station, and Institute of Atmospheric Physics, Chinese Academy of Sciences (IAP, CAS) (available from the corresponding author upon request), which provides data of the Beijing station. The OMPS/LP v2.5 stratospheric ozone profile product used for validation is available at https://ozoneaq.gsfc.nasa.gov/data/omps/#, accessed on 26 March 2021.

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