

# Simultaneous Column-Averaged CO<sub>2</sub>, Temperature, and HDO Measurement by Absorption Spectroscopy Lidar: Algorithm

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**Abstract**—Carbon dioxide (CO<sub>2</sub>) is the most important greenhouse gas in the atmosphere, playing a crucial role in the greenhouse effect and climate change. Lidar, with its high spatiotemporal resolution and high-precision detection capabilities, has become an essential tool for remote sensing of CO<sub>2</sub>. However, precise temperature information is required for CO<sub>2</sub> retrieval. Studies showed that for both differential absorption lidar (DIAL) and spectroscopic lidar, a CO<sub>2</sub> concentration measurement error of 2.0–3.5 ppm would result from each 1 K temperature deviation. Therefore, using nonreal-time and non in situ temperature data can lead to significant CO<sub>2</sub> retrieval errors. In this study, a column-averaged CO<sub>2</sub> spectroscopy lidar is proposed, which enables simultaneous measurements of CO<sub>2</sub> concentration, temperature, and semi-heavy water (HDO, isotopic water vapor). First, a model combining five Lorentzian functions with a binomial background was proposed through spectral decomposition. Second, through theoretical analysis, the fitting parameters were reduced from 18 to 5. Finally, theoretical analysis shows that the model achieves system biases of less than 0.1 ppm for CO<sub>2</sub>, 0.1 K for temperature, and 0.06 ppm for HDO. Considering Poisson noise, the error distributions of CO<sub>2</sub>, temperature, and HDO under different optical distances and signal-to-noise ratios (SNRs) were studied. This technology will advance the development of CO<sub>2</sub> flux remote sensing and is expected to play a crucial role in ecosystem research, atmospheric environmental monitoring, and greenhouse gas emission reduction policies.

**Index Terms**—Absorption spectroscopy, carbon dioxide (CO<sub>2</sub>) measurement, lidar, temperature measurement.

## I. INTRODUCTION

IN RECENT years, the increase in atmospheric carbon dioxide concentration ( $X_{\text{CO}_2}$ ) has drawn widespread attention. As of 2023, the global atmospheric average  $X_{\text{CO}_2}$  has exceeded 420 ppm, a significant rise from the preindustrial level of 280 ppm [1]. Studies have shown that for every 100 ppm increase in  $X_{\text{CO}_2}$ , the surface temperature of the Earth rises by approximately 1.5 °C [2], [3]. High  $X_{\text{CO}_2}$  leads to global warming, ocean acidification [4], biodiversity loss, and threats to human health [5]. Therefore, the accurate detection of  $X_{\text{CO}_2}$

is crucial for understanding and mitigating the impacts of climate change.

Existing in situ measurement techniques, such as high sensitivity cavity ring-down spectroscopy, can achieve remarkable  $X_{\text{CO}_2}$  measurement precision of 0.1 ppm [6]. However, since these in situ techniques require air sampling, they can only perform fixed-point measurements [6]. In contrast, CO<sub>2</sub> lidar technology enables remote sensing of  $X_{\text{CO}_2}$  with its high temporal and spatial resolution. Therefore, it is receiving increasing attention and has been applied in volcanic CO<sub>2</sub> flux measurements [7] and urban area CO<sub>2</sub> monitoring [8].

In the past decade, advancements in infrared detection technology and infrared laser technology have significantly improved the performance of CO<sub>2</sub> lidar. To improve detection sensitivity, a CO<sub>2</sub> lidar utilizing a superconducting nanowire single-photon detector (SNSPD) has been developed [9]. Additionally, a 1.57- $\mu\text{m}$  CO<sub>2</sub> lidar based on coherent detection has been designed to simultaneously measure wind speed and  $X_{\text{CO}_2}$  for flux measurements [10], [11]. To enhance CO<sub>2</sub> detection accuracy and enable the simultaneous measurement of multiple gases, such as H<sub>2</sub>O, a multiwavelength lidar system has also been introduced [12], [13]. Furthermore, airborne [14], [15] and spaceborne [16], [17] CO<sub>2</sub> lidars have been proposed to monitor CO<sub>2</sub> uptake over oceans and conduct global CO<sub>2</sub> surveys.

However, whether employing dual-wavelength differential absorption lidar (DIAL) systems or multiwavelength lidar systems, such as spectroscopy lidar systems, converting lidar backscattered signals to  $X_{\text{CO}_2}$  requires temperature data [18]. In other words, the precision of  $X_{\text{CO}_2}$  detection is directly influenced by the accuracy of temperature data. However, temperature data are typically obtained from radiosondes or models, which are nonreal time and nonin situ. These temperature data inevitably introduce errors in  $X_{\text{CO}_2}$  retrieval [19].

Conversely, the sensitivity of CO<sub>2</sub> lidar inversion to temperature implies the potential for simultaneously conducting temperature inversion [12], [13]. Unfortunately, research in this field is relatively limited. On the one hand, the lidar light source must emit enough wavelengths to capture the entire CO<sub>2</sub> absorption spectrum. On the other hand, there is a lack of inversion algorithms capable of simultaneously retrieving both  $X_{\text{CO}_2}$  and temperature [13], [19].

Meanwhile, once simultaneous measurements of  $X_{\text{CO}_2}$  and temperature are achievable, it will not only enhance the

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accuracy of lidar measurements of  $X_{\text{CO}_2}$  but also hold significant importance for calculating  $\text{CO}_2$  flux using the eddy covariance method [20]. This is because temperature has a significant impact on turbulent transport processes. Temperature variations can induce buoyancy effects that influence turbulence intensity, which in turn affects the transport and diffusion of  $\text{CO}_2$ . Additionally, temperature data are crucial for calculating sensible and latent heat fluxes, which help ensure energy balance closure and accurately distinguish the contribution of biological processes to  $\text{CO}_2$  flux [21].

In this study, a column-averaged  $\text{CO}_2$  spectroscopy lidar is proposed, which enables simultaneous measurements of  $X_{\text{CO}_2}$ , temperature, and HDO concentration ( $X_{\text{HDO}}$ ). First, the principle of  $\text{CO}_2$  lidar is described in detail, and then, the theoretical study of the errors in  $X_{\text{CO}_2}$  retrieval caused by temperature deviation ( $\Delta T$ ) in both DIAL and spectroscopy lidar is conducted. Then, the feasibility of using the  $\text{CO}_2$  absorption spectrum for simultaneous temperature retrieval is validated by analyzing the relationship between temperature parameters and absorption spectrum width. Subsequently, a model for the  $\text{CO}_2$  absorption spectrum is proposed, which utilizes a five-peak Lorentzian combined with a binomial background. To improve the fitting efficiency and accuracy, theoretical analysis was conducted to reduce the number of fitting parameters from 18 to only 5. Finally, numerical simulations verify the effectiveness of this algorithm and establish the relationship between the errors in  $X_{\text{CO}_2}$ , temperature, and  $X_{\text{HDO}}$  with the signal-to-noise ratio (SNR) and optical distance, thereby providing theoretical guidance for experimental research.

## II. PRINCIPLE OF $\text{CO}_2$ LIDAR

The backscattered photons received by the  $\text{CO}_2$  lidar at a distance of  $R$  can be expressed as [22]

$$N_s(x_i, R) = \frac{E \cdot 100}{h \cdot x_i} \eta_0 \eta_q \frac{A_t}{R^2} O(R) \frac{\tau}{2} \beta(x_i, R) T_r^2(x_i, R) \quad (1)$$

where  $N_s$  is the backscattered photon counts,  $E$  is the pulse energy (J),  $c$  is the speed of light,  $x_i$  is the laser wavenumber ( $\text{cm}^{-1}$ ),  $R$  is the distance (m),  $h$  is the Planck constant,  $\eta_0$  is the optical efficiency of the lidar system (%),  $\eta_q$  is the quantum efficiency (%),  $A_t$  is the effective area of the telescope ( $\text{m}^2$ ),  $O(R)$  is the geometric overlap factor at a distance of  $R$ ,  $\tau$  is the laser pulse duration (s),  $\beta$  represents the  $180^\circ \text{C}$  volume backscattering coefficient of aerosols ( $\text{m}^{-1}$ ), and  $T_r$  is the transmission term, which can be expressed as

$$T_r(x_i, R) = \exp\left\{-\int_0^R [\alpha_a(x_i, R) + \alpha_s(x_i, R)] dr\right\} \quad (2)$$

where  $\alpha_a$  is the extinction coefficient of aerosol ( $\text{m}^{-1}$ ),  $\alpha_s$  is the extinction coefficient of molecules and can be described as  $\alpha_s = \alpha + \alpha_m$ , where  $\alpha$  is the absorption coefficient of the gas under investigation and  $\alpha_m$  represents other extinction processes of molecules.

The  $\text{CO}_2$  lidar measures  $X_{\text{CO}_2}$  by detecting the absorption of laser signals by  $\text{CO}_2$  in the atmosphere. During the measurement process, since wavelength variations are generally within 0.2 pm,  $\beta$ ,  $\alpha_a$  and  $\alpha_m$  can be assumed to be wavelength-insensitive. Hence, the ratio of backscattered photon counts

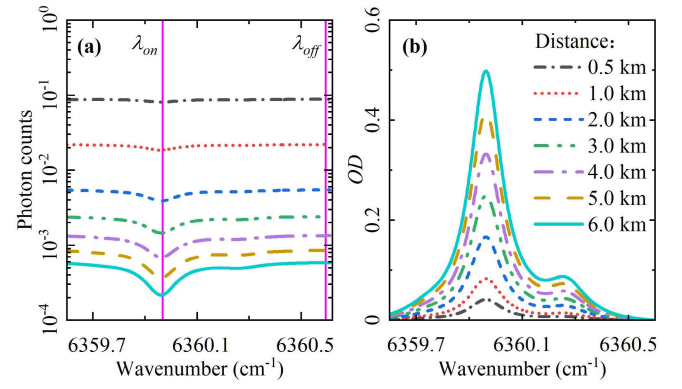


Fig. 1. (a) Spectra of backscattered photon counts  $N_s(x_i, R)$  and (b) total OD spectra of  $\text{CO}_2$  at various distances under 450-ppm  $\text{CO}_2$ , 5.28-ppm HDO, 297 K, and 1 atm.

between the two wavenumbers can be expressed as

$$\frac{N_{s_i}}{N_{s_0}} = \exp\left(-2 \int_0^R [\alpha_i - \alpha_0] dr\right) \quad (3)$$

where  $\alpha_i$  and  $\alpha_0$  are the  $\text{CO}_2$  absorption coefficient at the wavenumber of  $x_i$  and  $x_0$ , respectively.

In the  $6360\text{-cm}^{-1}$  spectral interval, with the weak  $\text{CO}_2$  absorption line at  $6360.60\text{ cm}^{-1}$  serving as a reference point, integrate the absorption coefficient from 0 to  $R$  to obtain the optical depth (OD), which is expressed as

$$\text{OD}(x_i, R) = -0.5 \ln\left[\frac{N_{s_i}}{N_{s_0}}\right] = \int_0^R [\alpha(x_i, R) - \alpha(x_0, R)] dr. \quad (4)$$

The photon counts  $N_s(x_i, R)$  in the  $6359.60\text{--}6360.60\text{ cm}^{-1}$  band can be reconstructed using (1), resulting in the relative spectra at different distances presented in Fig. 1. Utilizing the data from Fig. 1(a) and applying (4), the OD spectra at different distances can be calculated, as shown in Fig. 1(b). From Fig. 1, it is evident that both the photon count spectra and the OD spectra exhibit increased spectral contrast with increasing distance, which is beneficial for detection.

## III. IMPACT OF TEMPERATURE DEVIATION ON $\text{CO}_2$ CONCENTRATION RETRIEVAL

### A. Effect of Temperature Deviation on $\text{CO}_2$ DIAL

In  $\text{CO}_2$  DIAL, two laser wavelengths are typically used: one located at a strong  $\text{CO}_2$  absorption feature, referred to as the online ( $\lambda_{\text{on}}$ ), and another selected from a weak  $\text{CO}_2$  absorption band, known as the offline ( $\lambda_{\text{off}}$ ). By analyzing the intensity and distance information from the backscattered signal of a hard target, the column-averaged  $X_{\text{CO}_2}$  can be retrieved [23]. According to (4), the OD of DIAL can be expressed as

$$\text{OD} = -0.5 \ln\left[\frac{N_{\text{on}}}{N_{\text{off}}}\right] \quad (5)$$

where  $N_{\text{on}}$  is the photon count at  $\lambda_{\text{on}}$  and  $N_{\text{off}}$  is the photon count at  $\lambda_{\text{off}}$ . According to OD, the molecular number density of  $\text{CO}_2$   $N_{\text{CO}_2}$  (molecule/ $\text{m}^3$ ) in the atmosphere can be retrieved as

$$N_{\text{CO}_2} = \frac{\text{OD}}{(\sigma_{\text{on}} - \sigma_{\text{off}})R} \quad (6)$$

where  $\sigma_{\text{on}}$  is the absorption cross section of CO<sub>2</sub> at  $\lambda_{\text{on}}$  and  $\sigma_{\text{off}}$  is the absorption cross section at  $\lambda_{\text{off}}$ .

According to the ideal gas state equation, the number density of CO<sub>2</sub> ( $N_{\text{CO}_2}$ ) can be converted to  $X_{\text{CO}_2}$  [24]

$$X_{\text{CO}_2} = \frac{N_{\text{CO}_2}}{n} \times 10^6 = \frac{N_{\text{CO}_2} k_b T}{P} \times 10^6 \quad (7)$$

where  $n$  is the molecular number density of the atmosphere (molecule/m<sup>3</sup>),  $P$  is the ambient pressure (Pa),  $T$  is the ambient temperature (K), and  $k_b$  is Boltzmann's constant.

From the above analysis, the impact of temperature deviation  $\Delta T$  on  $X_{\text{CO}_2}$  involves two aspects: first, temperature affects the calculation of  $N_{\text{CO}_2}$  in the process of retrieving  $X_{\text{CO}_2}$  [as indicated in (7)]; secondly, the CO<sub>2</sub> absorption cross section, which is necessary for calculating  $N_{\text{CO}_2}$  as described in (6), also depends on temperature data. To simultaneously consider both factors, Han et al. [25] introduced a weighting factor ( $w$ ) to comprehensively account for the influence, which can be expressed as

$$w = \frac{\sigma_{\text{on}} - \sigma_{\text{off}}}{k_b T / P}. \quad (8)$$

Thus, (7) can be rewritten as

$$X_{\text{CO}_2} = \frac{1}{2wR} \cdot \ln \frac{N_{\text{on}}}{N_{\text{off}}}. \quad (9)$$

To quantitatively analyze the error of  $X_{\text{CO}_2}$  ( $\Delta X_{\text{CO}_2}$ ) caused by  $\Delta T$ , this work carried out the following studies: 1) the deviation in the absorption cross section caused by  $\Delta T$  leads to errors in  $X_{\text{CO}_2}$  retrieval; 2) when converting  $N_{\text{CO}_2}$  to  $X_{\text{CO}_2}$ , as indicated by (7), the impact of  $\Delta T$  on  $X_{\text{CO}_2}$  retrieval; and 3) the combined effect of the above two factors on  $X_{\text{CO}_2}$  retrieval, as shown in (9).

The results from these analyses are shown in Fig. 2. During the simulation process,  $X_{\text{HDO}}$  was set to 5.28 ppm and pressure to 1 atm. The  $\Delta X_{\text{CO}_2}$  introduced by  $\Delta T$  when calculating the absorption cross section is shown in Fig. 2(a). That is, assuming there is no temperature deviation when calculating  $X_{\text{CO}_2}$  using (7), while a temperature deviation is present in calculating  $N_{\text{CO}_2}$  using (6), resulting in  $\Delta X_{\text{CO}_2}$ . For every 1 K deviation in temperature, the  $\Delta X_{\text{CO}_2}$  increases by 0.68–1.23 ppm. Higher  $X_{\text{CO}_2}$  and higher temperatures result in larger  $\Delta X_{\text{CO}_2}$ . The  $\Delta X_{\text{CO}_2}$  caused by  $\Delta T$  when converting  $N_{\text{CO}_2}$  to  $X_{\text{CO}_2}$  is shown in Fig. 2(b). That is, assuming there is no temperature deviation when calculating  $N_{\text{CO}_2}$  using (6), while a temperature deviation is present in calculating  $X_{\text{CO}_2}$  using (7), resulting in  $\Delta X_{\text{CO}_2}$ . In this case, for every 1 K deviation in temperature, the  $\Delta X_{\text{CO}_2}$  increases by 1.18–2.22 ppm. Furthermore, higher  $X_{\text{CO}_2}$  and lower temperatures result in larger  $\Delta X_{\text{CO}_2}$ . The combined effect of  $\Delta T$  on  $\Delta X_{\text{CO}_2}$ , calculated by (9), is shown in Fig. 2(c). That is, assuming temperature deviation exists both in calculating  $X_{\text{CO}_2}$  using (7) and in calculating  $N_{\text{CO}_2}$  using (6), resulting in  $\Delta X_{\text{CO}_2}$ . As illustrated in Fig. 2(c), the impact of  $\Delta T$  on  $\Delta X_{\text{CO}_2}$  varies with different atmospheric temperatures and  $X_{\text{CO}_2}$  levels. For every 1 K deviation in temperature,  $\Delta X_{\text{CO}_2}$  increases by approximately 1.96–3.28 ppm. Overall, higher  $X_{\text{CO}_2}$  and lower temperatures lead to larger  $\Delta X_{\text{CO}_2}$ .

TABLE I  
PARAMETERS OF THE FIVE ABSORPTION PEAKS USED  
IN THE MODEL [29]

Formula	<sup>12</sup> C <sup>16</sup> O <sub>2</sub>	HD <sup>16</sup> O	HD <sup>16</sup> O	<sup>12</sup> C <sup>16</sup> O <sub>2</sub>	<sup>12</sup> C <sup>16</sup> O <sub>2</sub>
Peak number	S <sub>1</sub>	S <sub>2</sub>	S <sub>3</sub>	S <sub>4</sub>	S <sub>5</sub>
AFGL code	626	162	162	626	626
$x_0$	6359.967	6359.748	6360.278	6360.113	6359.864
$S(T_0)$	$1.76 \times 10^{-23}$	$2.22 \times 10^{-26}$	$8.62 \times 10^{-26}$	$3.01 \times 10^{-25}$	$4.90 \times 10^{-26}$
$\gamma_{\text{air}}$	0.0740	0.0970	0.0954	0.0847	0.0730
$\gamma_{\text{self}}$	0.100	0.394	0.448	0.116	0.098
$E''$	106.1297	362.5072	100.3909	675.2049	1521.615
$n_{\text{air}}$	0.70	0.79	0.79	0.69	0.70
$P_{\text{self}}$	-0.00563	-0.00786	-0.01346	-0.00374	-0.00585
abundance	0.984204	0.000311	0.000311	0.984204	0.984204

### B. Effect of Temperature Deviation on CO<sub>2</sub> Spectroscopy Lidar

DIAL cannot obtain the full absorption spectrum information of CO<sub>2</sub> because it uses only two wavelengths. To address this limitation, Yu et al. [13] proposed a scheme in 2021 to acquire the CO<sub>2</sub> absorption spectrum, enabling the retrieval of multiple gases, including CO<sub>2</sub> and HDO. To decompose the absorption spectrum CO<sub>2</sub>, a model was proposed for nonlinear least squares fitting of the OD spectrum. The model employs three Lorentzian functions, namely,  $S_1$ – $S_3$  (see Table I), to represent the three strongest absorption peaks around 6359.96 cm<sup>-1</sup>, along with a constant background value ( $B$ ), which can be expressed as follows:

$$F(x) = f_1(x) + f_2(x) + f_3(x) + B \quad (10)$$

where  $f_i(x)$  represents a Lorentzian function, which can be expressed as

$$f_i(x) = \frac{A_i}{\pi} \frac{\omega_{Li}}{\omega_{Li}^2 + (x - x_{ci})^2} \quad (i = 1, 2, 3) \quad (11)$$

where  $A$  is the area of the Lorentzian peak (cm<sup>-2</sup>),  $\omega_L$  is the half-width at half-maximum (HWHM) of the Lorentzian function (cm<sup>-1</sup>), and  $x_c$  is the central wavenumber of the Lorentzian function under ambient conditions (cm<sup>-1</sup>).

To obtain distance-resolved OD, the OD is transformed into unit OD (UOD) before performing the fitting as follows:

$$\text{UOD}(x_i, R) = -\frac{1}{2R} \ln \left[ \frac{N_{s_i}}{N_{s_0}} \right] = \alpha(x_i, R) - \alpha(x_0, R). \quad (12)$$

In the near-Earth atmospheric environment, the line shape of the absorption peak is the Lorentz line shape [26]. The absorption coefficient at the wavenumber is equal to the sum of the absorption coefficients of all absorption peaks at this wavenumber

$$\alpha(x) = \sum f(x) \quad (13)$$

where  $f(x)$  represents a Lorentzian function, as described by (11).



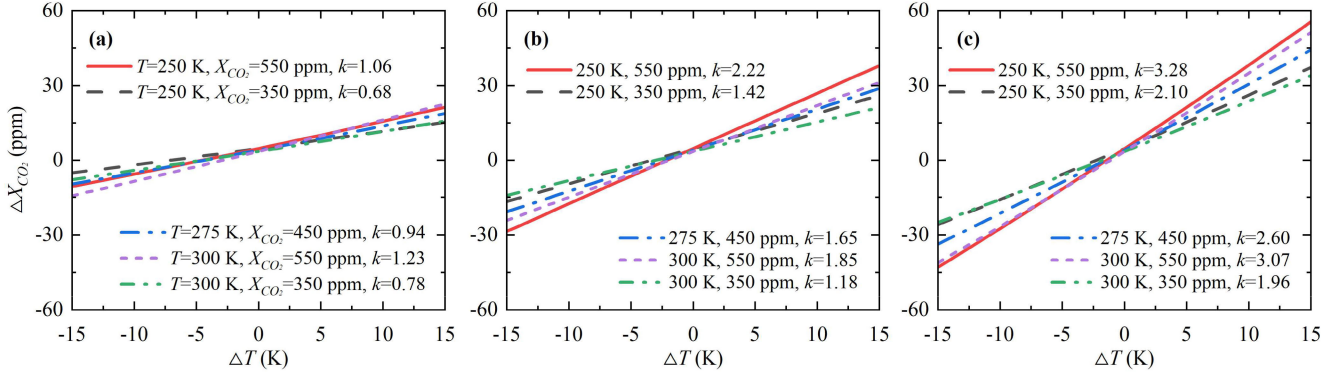


Fig. 2. Analysis of  $X_{CO_2}$  retrieval errors ( $\Delta X_{CO_2}$ ) caused by temperature deviation ( $\Delta T$ ) in DIAL. (a)  $\Delta X_{CO_2}$  resulting from the absorption cross section deviation due to temperature deviation. (b)  $\Delta X_{CO_2}$  resulting from  $\Delta T$  when converting  $N_{CO_2}$  to  $X_{CO_2}$ . (c)  $\Delta X_{CO_2}$  caused by  $\Delta T$  under the combined effect of the two factors mentioned above. (The parameter  $k$  in the figure represents the slope of the  $\Delta T$  versus  $\Delta X_{CO_2}$  curve, indicating the error in  $\Delta X_{CO_2}$  retrieval for each 1 K deviation).

The area  $A$  of the Lorentzian profile is fitted to UOD for the retrieval of  $CO_2$  and  $HDO$  concentrations, where  $A$  can be expressed as

$$A = \frac{S(T)P_{\text{self}}}{k_b T \times 10^6} \quad (14)$$

where  $P_{\text{self}}$  represents the partial pressure of the target gas, which can be expressed as

$$P_{\text{self}} = P \cdot X \cdot \text{abundance} \quad (15)$$

where  $X$  is the concentration of the target gas, abundance refers to the natural abundance of the target isotope in the environment, and  $S(T)$  represents the spectral line intensity at temperature  $T$  (cm/molecule), which can be expressed as [27]

$$S(T) = S(T_0) \frac{Q(T_0)}{Q(T)} \left\{ \frac{1 - \exp(-c_2 x_0/T)}{1 - \exp(-c_2 x_0/T_0)} \right\} \exp \left[ E'' c_2 \left( \frac{1}{T_0} - \frac{1}{T} \right) \right] \quad (16)$$

$$c_2 = \frac{h \times c}{k_b} = 1.4387769 \text{ cm} \cdot \text{K} \quad (17)$$

$$x_c = x_0 + P \times P_{\text{shift}} \times \left( \frac{T_0}{T} \right)^{n_{\text{air}}} \quad (18)$$

where  $S(T_0)$  is the spectral line intensity at  $T_0$  (cm/molecule),  $x_0$  is the wavenumber of the spectral line transition ( $\text{cm}^{-1}$ ) in vacuum,  $Q(T_0)$  is the total internal partition sum at  $T_0$  and can be downloaded from HITRAN2020,  $Q(T)$  is the total internal partition sum at  $T$ ,  $c_2$  is the second radiation constant, and  $E$  is the lower state energy of the transition ( $\text{cm}^{-1}$ ).

Finally, the concentration of the target gas  $X$  can be expressed as

$$X = \frac{A}{S(T)n_L} \frac{P_0}{P} \frac{T}{T_0} \quad (19)$$

where  $P_0$  is 1 atm,  $T_0$  is 296 K, and  $n_L$  (molecule/ $\text{m}^3$ ) denotes the molecular number density in the atmosphere under the conditions of  $P_0$  and  $T_0$ . Additionally, when the concentration of  $CO_2$  is expressed in ppm, the  $CO_2$  concentration needs to be multiplied by  $10^6$ . Similarly, the  $HDO$  concentration needs to be multiplied by  $10^6$  since  $HDO$  is expressed in ppm.

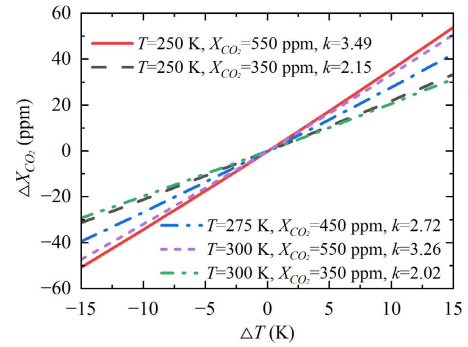


Fig. 3. Effect of temperature deviation on spectroscopy lidar to measure  $CO_2$ .

However, it is still necessary to incorporate the temperature information in the retrieval process. The deviation in temperature will lead to errors in the retrieval of  $X_{CO_2}$  and  $X_{HDO}$ . Assuming other parameters are known and based on the model described in (10), the  $\Delta X_{CO_2}$  caused by the temperature deviation when using (11)–(19) is shown in Fig. 3. Calculations show that every 1 K deviation in temperature will lead to a 2.02–3.49-ppm deviation in  $CO_2$ . However, it is challenging to obtain synchronized and accurate temperature data in experiments. Therefore, obtaining temperature data simultaneously while measuring  $CO_2$  is particularly important.

#### IV. FEASIBILITY ANALYSIS OF TEMPERATURE RETRIEVAL VIA ABSORPTION SPECTROSCOPY

The width  $\omega_L$  of the absorption spectrum of  $CO_2$  is affected by temperature, and its width can be expressed as [27]

$$\omega_L = \left( \frac{T_0}{T} \right)^{n_{\text{air}}} \left[ \gamma_{\text{air}}(P_0, T_0)(P - P_{\text{self}}) + \gamma_{\text{self}}(P_0, T_0)P_{\text{self}} \right] \quad (20)$$

where  $n_{\text{air}}$  is the coefficient of the temperature dependence of  $\omega_L$ ,  $P_{\text{shift}}$  is the pressure shift at the spectral line position ( $\text{cm}^{-1}/\text{atm}$ ), and  $\gamma_{\text{air}}$  and  $\gamma_{\text{self}}$  are the air-broadened  $\omega_L$  ( $\text{cm}^{-1}/\text{atm}$ ) and self-broadened  $\omega_L$  ( $\text{cm}^{-1}/\text{atm}$ ) at  $T_0$  and  $P_0$ , respectively.

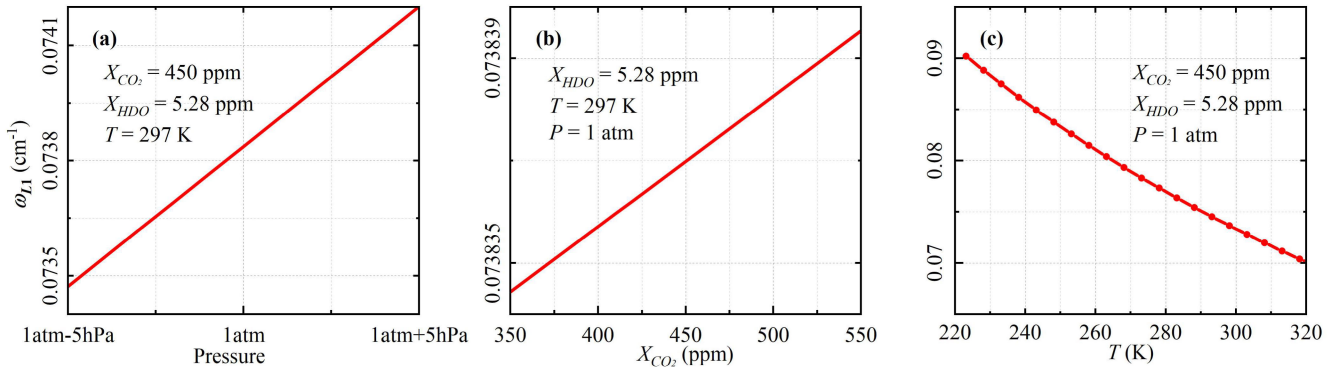


Fig. 4. Effects of (a) pressure, (b)  $X_{\text{CO}_2}$ , and (c) temperature on  $\omega_L$ .

As indicated in (20),  $P$ ,  $P_{\text{self}}$ , and  $T$  codetermine  $\omega_L$ . The influence of these three parameters on  $\omega_L$  will be analyzed individually. First, the atmospheric pressure profile is relatively stable in the vertical direction, allowing the use of model data with deviations within  $\pm 2$  hPa [28]. Fig. 4(a) shows that under 1 atm, variations in  $\omega_L$  remain within 1% when pressure deviates by  $\pm 5$  hPa. Therefore, although  $P$  influences the magnitude of  $\omega_L$ , accurate pressure data can minimize the error it introduced. Additionally, the influence of  $P_{\text{self}}$  on  $\omega_L$  is approximately in the range of  $10^{-5}$ – $10^{-4}$  of its own magnitude and can therefore be neglected. In (20),  $\gamma_{\text{air}}(P_0, T_0)(P - P_{\text{self}})$  represents the contribution of pressure from other gases in the atmosphere to  $\omega_L$  broadening, while  $\gamma_{\text{air}}(P_0, T_0)P_{\text{self}}$  represents the contribution of partial pressure from the target gas to  $\omega_L$  broadening. Fig. 4(b) shows that when  $X_{\text{CO}_2}$  changes from 350 to 550 ppm at  $T_0$  and  $P_0$ ,  $\omega_L$  increased by only  $5 \times 10^{-6} \text{ cm}^{-1}$ . Additionally, the analysis of  $\omega_L$  in  $S_2$  revealed that when  $X_{\text{HDO}}$  increased from 3.11 to 6.21 ppm,  $\omega_L$  increased by only  $9 \times 10^{-7} \text{ cm}^{-1}$ , indicating that the magnitude of the variable itself is approximately  $10^{-2} \text{ cm}^{-1}$ . The above analysis indicates that  $\omega_L$  is minimally affected by changes in gas concentration.

In contrast,  $\omega_L$  is much more sensitive to temperature changes than to variations in gas concentration. According to (20), the width of the CO<sub>2</sub> absorption peak  $S_1$ ,  $\omega_L$ , can be calculated as the temperature changes from 223 to 324 K. The results are shown in Fig. 4(c), where  $\omega_L$  changes by approximately  $2.5 \times 10^{-4} \text{ cm}^{-1}$  for every 1 K change in temperature. This indicates that  $\omega_L$  is sensitive to temperature variations. In summary,  $\omega_L$  is minimally affected by gas concentration and is primarily determined by temperature. This provides a basis for using  $\omega_L$  for temperature retrieval.

However, the three-peak Lorentzian plus background model described by (10) is insufficient for accurately describing CO<sub>2</sub> absorption spectra. As shown in Fig. 5, with  $X_{\text{CO}_2}$  set to 450 ppm,  $X_{\text{HDO}}$  set to 5.28 ppm, pressure at 1 atm, and temperature at 297 K, the systematic errors from least-squares fitting using (10) are evident. Fig. 5(a) shows that as  $X_{\text{CO}_2}$  increases from 350 to 550 ppm, the systematic error of  $X_{\text{CO}_2}$  rises from 8.5 to 12.7 ppm. Fig. 5(b) indicates that for temperature inversion from 250 to 310 K, the deviation between true and inverted temperatures follows a quadratic function, peaking at 270 K with an error of 4.36 K, decreasing

but still above 4.15 K on either side. Fig. 5(c) reveals that the  $X_{\text{HDO}}$  bias is minimized at 4.66 ppm, increasing on both sides. Thus, to improve accuracy, it is necessary to develop a model that more accurately approximates the real absorption spectrum.

## V. DETERMINATION OF THE ABSORPTION SPECTRUM MODEL

### A. Spectral Decomposition

To accurately describe the absorption spectrum of CO<sub>2</sub>, the absorption spectrum needs to be decomposed first. Fig. 6(a) shows the absorption spectrum calculated using data from the HITRAN2020 database [29]. Using the criterion of peak intensities being more than twice as strong as other background absorption peaks, five absorption peaks, labeled  $S_1$  through  $S_5$ , are selected, with their locations shown in Fig. 6(a). According to the HITRAN database, the peak positions of these five absorption peaks are 6359.967, 6359.748, 6360.278, 6360.113, and 6359.864  $\text{cm}^{-1}$ . In atmospheric CO<sub>2</sub> detection, the influence of atmospheric pressure and temperature on these peak positions is negligible. However, Doppler shifts caused by atmospheric wind speed do affect them. Fortunately, the Doppler-induced frequency shift can be compensated for by adding a wind measurement function to the CO<sub>2</sub> lidar [30]. When the three peaks  $S_1$ – $S_3$ , as shown in (10), are subtracted from the spectrum, the resulting spectrum is shown in Fig. 6(b). As shown there, this resulting spectrum cannot be solely represented by the background constant  $B$  in (10). This discrepancy is the reason why using (10) to describe the absorption spectrum results in significant systematic deviations in  $X_{\text{CO}_2}$ , temperature, and  $X_{\text{HDO}}$ , as shown in Fig. 5.

From Fig. 6(b), it can be observed that peak  $S_4$  has a significant impact on the background. After subtracting  $S_4$ , the remaining absorption spectrum is shown as the dashed line in Fig. 6(c), and peak  $S_5$  still stands out in the remaining spectrum. After subtracting  $S_5$ , the residual spectrum, shown as the solid line in Fig. 6(c), reveals that the residual background curve can be represented by a binomial. Therefore, to enhance the representation of the absorption spectrum, a model is introduced that describes the CO<sub>2</sub> absorption spectrum using a five-peak Lorentzian combined with a binomial background,

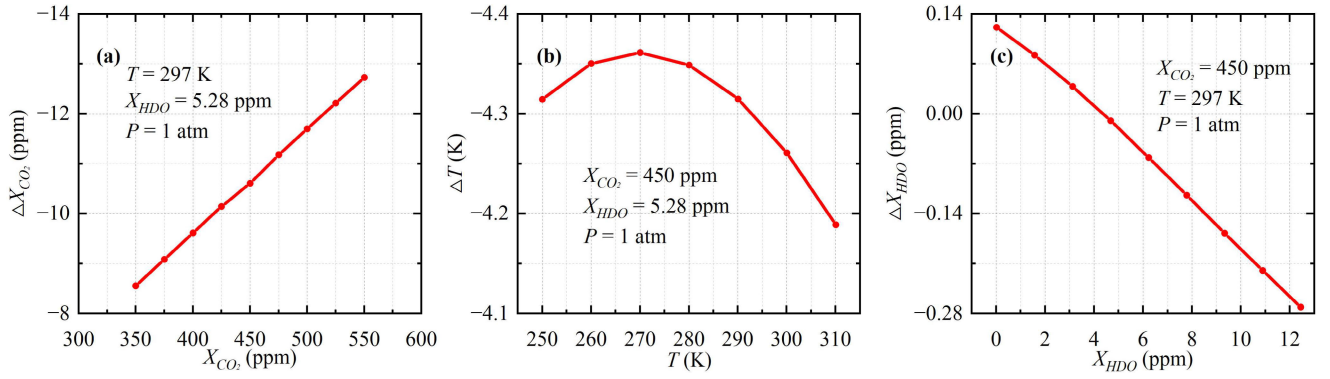


Fig. 5. Systematic errors introduced by the three-peak model described in (10) for (a) CO<sub>2</sub> concentration, (b) temperature, and (c) HDO concentration.

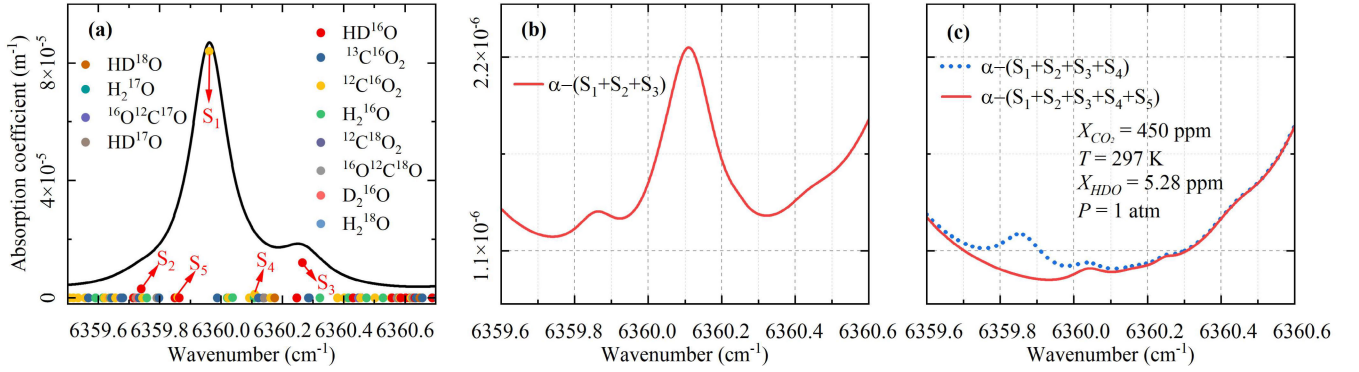


Fig. 6. (a) Absorption spectrum in the 6360-cm<sup>-1</sup> band. (b) Residual spectrum after removing peaks S<sub>1</sub>–S<sub>3</sub>. (c) Residual spectrum (solid line) after removing peaks S<sub>1</sub>–S<sub>4</sub>, and the residual spectrum (dashed line) after removing S<sub>1</sub>–S<sub>5</sub>.

as shown in the following:

$$F(x) = f_1 + f_2 + f_3 + f_4 + f_5 + a_B(x - b_B)^2 + c_B. \quad (21)$$

The detailed parameters of the five absorption peaks used in the model are listed in Table I.

### B. Simplification of Fitting Parameters

However, when the model is updated from three Lorentz functions plus a background, as described in (10), to five Lorentz functions plus a binomial background, as described in (21), the number of unknown parameters to be determined increases to 18. This will significantly increase the difficulty of fitting and reduce its accuracy. Therefore, it is important to find relationships among the parameters in order to reduce the number of variables that need to be decided. First, the central positions of the five Lorentz functions need to be determined. As shown in (18), the central wavenumber is influenced by temperature and pressure. A change of 1 K in temperature results in a change of approximately  $1.5 \times 10^{-5}$  cm<sup>-1</sup> in the central wavenumber. Similarly, a change of 1 hPa in pressure leads to a change of approximately  $5.7 \times 10^{-8}$ . Therefore, these variations are negligible compared to the central wavenumber itself. Without considering the spectral shift caused by atmospheric wind speed [30], the central wavenumbers of the five Lorentz functions can be treated as known constants, with their specific values presented in Table I. Through the above analysis, the number of fitting

8 to 13. Second, parameter is reduced from 1, as shown in (14), area  $A$  is related to gas concentration and spectral line intensity  $S(T)$ . For the same gas, area  $A$  depends solely on the spectral line intensity  $S(T)$ . According to (16), the ratio between different peaks of the same gas depends only on the parameters of the absorption peaks themselves and the temperature. When the ambient temperature changes, the ratio of each peak area is shown in Fig. 7. For every 1 K increase in temperature, the  $A_3/A_2$  ratio decreases by about  $1.67 \times 10^{-3}$ , the  $A_4/A_1$  ratio increases by about  $1.59 \times 10^{-5}$ , and the  $A_5/A_1$  ratio increases by about  $6.40 \times 10^{-6}$ . Therefore, for the same gas, the area ratios between different peaks can be determined by temperature. In the fitting processes, once the temperature is determined, the ratios of  $A$  can be accordingly established. Furthermore, since the ratio of the areas of different peaks for the same gas can be obtained from the temperature, the three unknowns for the CO<sub>2</sub> peak areas, namely,  $A_1$ ,  $A_4$ , and  $A_5$ , are simplified to just one. Similarly, the two unknowns for the HDO peak areas,  $A_2$  and  $A_3$ , are simplified to one. Moreover, according to the analysis in Section IV,  $\omega_L$  is mainly affected by temperature rather than gas concentration. Therefore, the  $\omega_L$  values of the five Lorentz functions can be related through temperature. Calculated according to (20), the ratios of  $\omega_{L2}$ ,  $\omega_{L3}$ ,  $\omega_{L4}$ , and  $\omega_{L5}$  to  $\omega_{L1}$  with respect to temperature are shown in Fig. 8. From the picture, the ratios of each width to  $\omega_{L1}$  change slightly between 250 and 310 K. For every 1 K increase, the  $\omega_{L2}/\omega_{L1}$  ratio decreases by about  $3.97 \times 10^{-4}$ , the  $\omega_{L3}/\omega_{L1}$  ratio decreases by about  $3.90 \times 10^{-4}$ , the  $\omega_{L4}/\omega_{L1}$



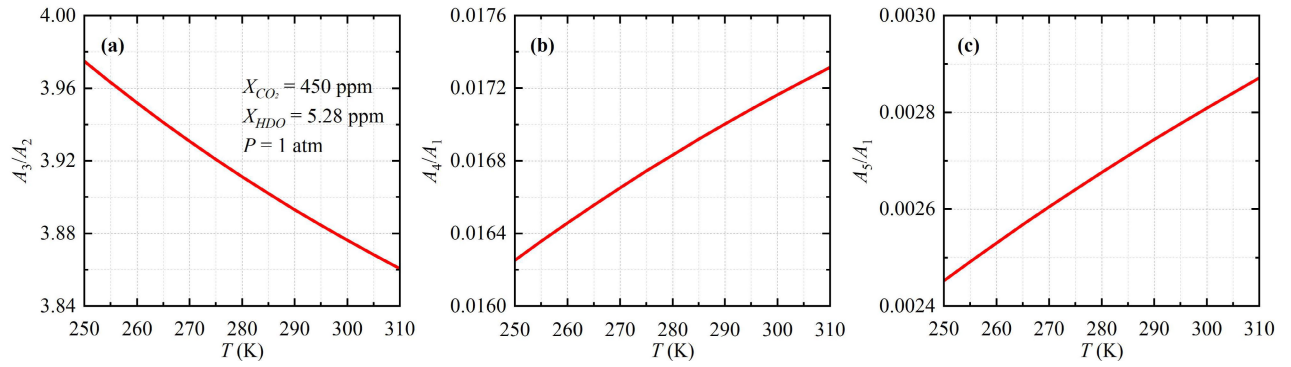


Fig. 7. Effect of temperature on the ratio of the area of absorption peaks (a)  $S_3$  and  $S_2$ ,  $A_3/A_2$ , (b)  $S_4$  and  $S_1$ ,  $A_4/A_1$ , and (c)  $S_5$  and  $S_1$ ,  $A_5/A_1$ .

ratio increases by about  $3.85 \times 10^{-5}$ , and the  $\omega_{L5}/\omega_{L1}$  ratio remains constant at 0.9865. This indicates that the ratios of the widths of the different absorption peaks to  $\omega_{L1}$  can be considered constants. Therefore, determining  $\omega_{L1}$  for the CO<sub>2</sub> absorption peak  $S_1$  as the only unknown is sufficient to determine the  $\omega_L$  values for the other four absorption peaks. Finally, a study on the model background was conducted. By analyzing the residual background spectra after subtracting the absorption spectra of  $S_1$ – $S_5$  under different CO<sub>2</sub> concentrations, HDO concentrations, temperatures, and pressures, it was found that these background values can be accurately fitted using a quadratic equation  $a_B(x - b_B)^2 + c_B$ . The results are shown in Fig. 9. Fig. 9(a) shows the background spectra for varying CO<sub>2</sub> concentrations. Fig. 9(b) presents the background spectra for different HDO concentrations. Fig. 9(c) illustrates the background spectra under different temperature, and Fig. 9(d) displays the background spectra at various temperatures. As shown in Fig. 9, the background spectra under different conditions can be well fitted using a univariate quadratic equation, with Fig. 9(a) illustrating an example of the fitting results. The analysis of these spectra reveals that the value of  $b_B$  consistently regresses to 6359.97, so  $b_B$  can be fixed as a constant 6359.97. This analysis reduces the number of unknowns in the background from three to two. Additionally, based on the results from Fig. 9, the initial values for  $a_B$  and  $c_B$  in the fitting are set to  $1.8 \times 10^{-6}$  and  $1.26 \times 10^{-5}$ . Based on the above analysis, the newly proposed absorption spectrum model, as represented by (21), simplifies the number of unknowns from 18 to 5. These five parameters are the area  $A_1$  of absorption peak  $S_1$ , the area  $A_2$  of absorption peak  $S_2$ , the  $\omega_{L1}$  of absorption peak  $S_1$ , and the background parameters  $a$  and  $c$ . Among these,  $A_1$  will be used to retrieve CO<sub>2</sub> concentration  $X_{CO_2}$ ,  $A_2$  will be used to retrieve HDO concentration  $X_{HDO}$ , and  $\omega_{L1}$  will be used to retrieve temperature.

### C. Model Verification

To verify the proposed model (21) and assess the feasibility of the simplified fitting parameters, a simulation and model validation study was carried out. First, the CO<sub>2</sub> absorption spectra in the range of 6359.60–6360.60 cm<sup>-1</sup> were selected. Thirty wavenumbers were chosen using uniform sampling, with 6360.60 cm<sup>-1</sup> set as the reference point. The UOD was

calculated according to (4) and (12). Subsequently, nonlinear fitting of the UOD was carried out using (10) and (21), respectively. The  $X_{CO_2}$  was set at 450 ppm,  $X_{HDO}$  at 5.28 ppm,  $P$  at 1 atm, and  $T$  at 297 K. Initial values for fitting were computed based on these environmental parameters. After the first fitting process was completed, the fitted results were used as initial values for the next fitting until the results of the fitting parameters stabilized. The fitting results of the newly proposed model and the model represented by (10) are shown in Fig. 10. During the computation, the absorption depth was set to 5 km. The analysis of the residuals in Fig. 10(b) and (d) reveals that the newly proposed model performs better, with residuals on the order of  $10^{-8}$ , which is an order of magnitude lower than those of the model described by (10). Subsequently, similar to Fig. 5, the five-peak model was applied under different environmental parameters to investigate its systematic errors. As shown in Fig. 11, with  $X_{CO_2}$  set to 450 ppm,  $X_{HDO}$  set to 5.28 ppm, pressure at 1 atm, and temperature at 297 K, the systematic errors from least-squares fitting using (21) are significantly reduced. For  $X_{CO_2}$  retrieval, it is found that the systematic errors of the five-peak model are less than 0.1 ppm across the range of  $X_{CO_2}$  from 350 to 550 ppm, as shown in Fig. 11(a). Fig. 11(b) shows that for temperature inversion from 250 to 310 K, the temperature deviation is less than 0.11 K, with the minimum error point located at 270 K. For  $X_{HDO}$  retrieval, the systematic error increases gradually with the HDO concentration varying from 0 to 12.43 ppm, but the maximum value remains below 0.06 ppm, as shown in Fig. 11(c). These results validate the effectiveness of the new model.

## VI. SIMULATION ANALYSIS

To validate the performance of the new model in a noisy environment, a simulation study was conducted. Since the CO<sub>2</sub> lidar system uses a single-photon detection scheme, its primary noise sources include shot noise (i.e., Poisson noise), solar radiation noise, and detector dark noise. For solar radiation noise, the lidar operates in the near-infrared range, where solar noise is minimal, allowing a narrowband filter to effectively suppress it. Regarding dark noise, current single-photon detection technologies, such as SNSPD, can achieve ultralow system dark count rates [13]. Therefore, this study considers only Poisson noise in the simulation. The specific simulation steps are as follows.

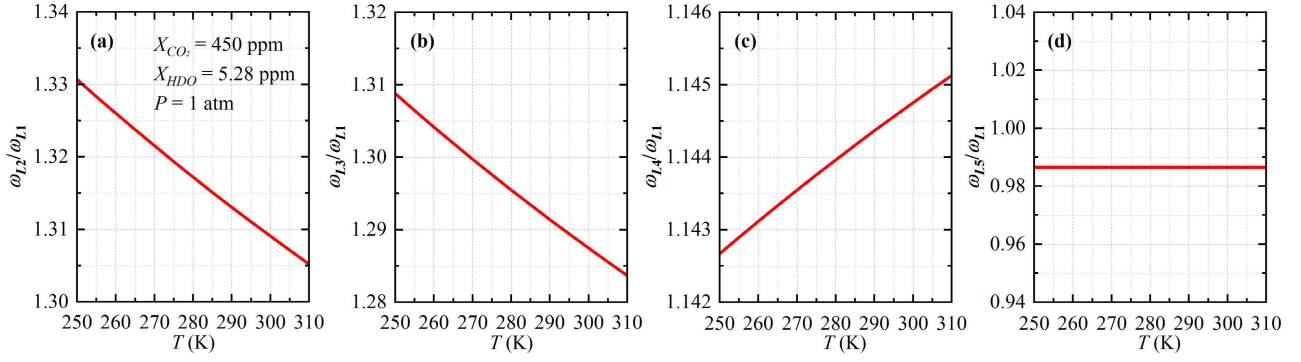


Fig. 8. Effect of temperature on the ratio of  $\omega_L$  for absorption peaks. (a)  $S_2$  and  $S_1$ , (b)  $S_3$  and  $S_1$ , (c)  $S_4$  and  $S_1$ , and (d)  $S_5$  and  $S_1$ .

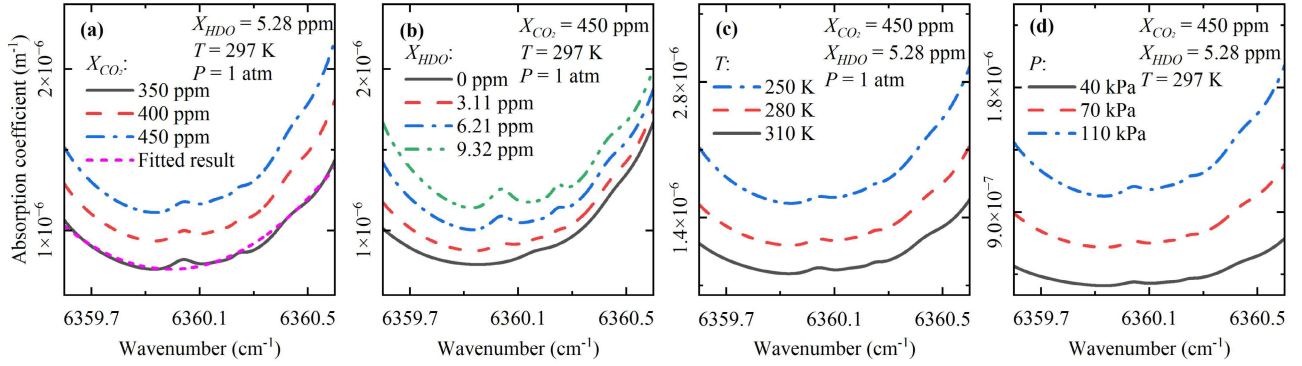


Fig. 9. (a)  $\text{CO}_2$  concentration, (b) HDO concentration, (c) temperature, and (d) pressure on the background spectra after removing the five absorption peaks.

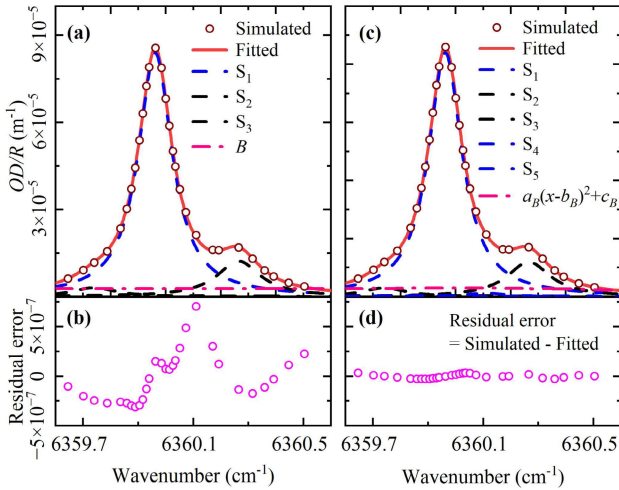


Fig. 10. Fitting results for (a) three-peak model and (c) five-peak model, with corresponding residual error shown in (b) and (d).

**Step 1:** Calculate the absorption coefficients for 30 wavenumbers uniformly distributed across the spectrum in the range of  $6359.60\text{--}6360.60\text{ cm}^{-1}$ , based on the atmospheric environment and gas concentrations [13]. During the simulation process, three different environmental conditions were considered: temperature 250 K with a  $\text{CO}_2$  concentration of 350 ppm; temperature 297 K with a  $\text{CO}_2$  concentration of 450 ppm; and temperature 300 K with a  $\text{CO}_2$  concentration of 550 ppm. In all cases, HDO is 5.28 ppm, and  $P$  is 1 atm.

**Step 2:** Simulate the backscattered photon counts at different wavenumbers and distances  $R$  using (3), based on specified detection SNR and incorporate Poisson noise into the simulated photon counts. Note that the SNR refers to the SNR at  $6360.60\text{ cm}^{-1}$ .

**Step 3:** Calculate the UOD according to (4) and (12).

**Step 4:** Perform nonlinear fitting on the simulated UOD using the five-peak Lorentzian model, as described by (21). The initial values of the fitting parameters,  $A_1$ ,  $A_2$ , and  $\omega_L$ , were calculated based on the following environmental conditions:  $X_{\text{CO}_2}$  at 450 ppm,  $X_{\text{HDO}}$  at 5.28 ppm,  $P$  at 1 atm, and  $T$  at 297 K.

**Step 5:**  $X_{\text{CO}_2}$ ,  $X_{\text{HDO}}$ , and  $T$  were calculated using the fitting parameters  $A_1$ ,  $A_2$ , and  $\omega_L$ , respectively.

**Step 6:** The initial retrieval results for  $X_{\text{CO}_2}$ ,  $X_{\text{HDO}}$ , and  $T$  calculated in Step 5 are used as the starting values for the next fitting. The iteration stops when the variance of  $X_{\text{CO}_2}$  in three consecutive iterations is less than  $10^{-9}$ .

**Step 7:** Backscattered signal spectra are generated under different SNRs (ranging from  $10^2$  to  $10^4$ , with intervals of 500) and varying detection distances (ranging from 1 to 10 km, with 1-km intervals). Additionally, Poisson noise is added to each signal spectrum to generate 100 independent sets of data, and Steps 2–6 are repeated to obtain 100 sets of  $X_{\text{CO}_2}$ ,  $X_{\text{HDO}}$ , and  $T$ . Finally, the standard deviation of these 100 sets is then calculated and denoted as  $\Delta X_{\text{CO}_2}$ ,  $\Delta X_{\text{HDO}}$ , and  $\Delta T$ , respectively.

To obtain analytical expressions for  $\Delta X_{\text{CO}_2}$ ,  $\Delta X_{\text{HDO}}$ , and  $\Delta T$  with respect to SNR and  $R$ , the data underwent the following statistical analysis. Taking the retrieval of  $\Delta X_{\text{CO}_2}$



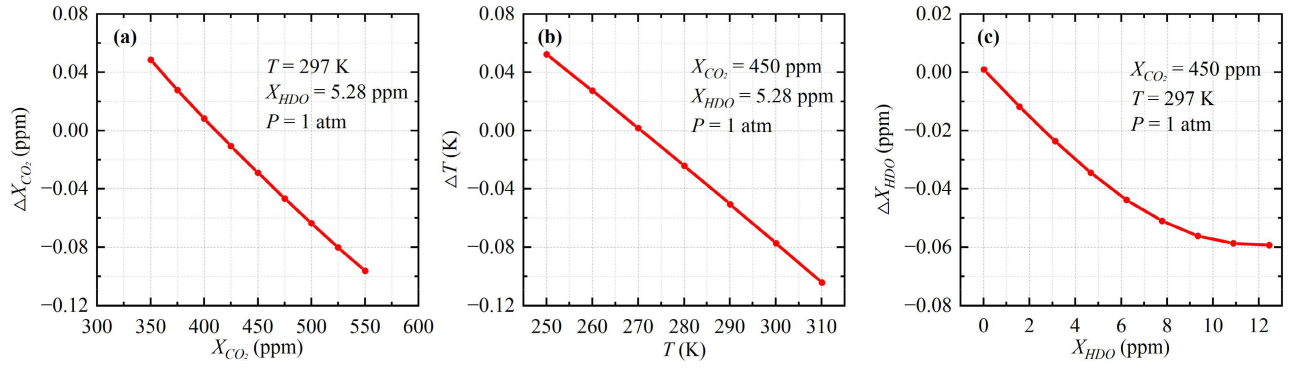


Fig. 11. Systematic errors introduced by the five-peak model described in (21) for (a) CO<sub>2</sub> concentration, (b) temperature, and (c) HDO concentration.

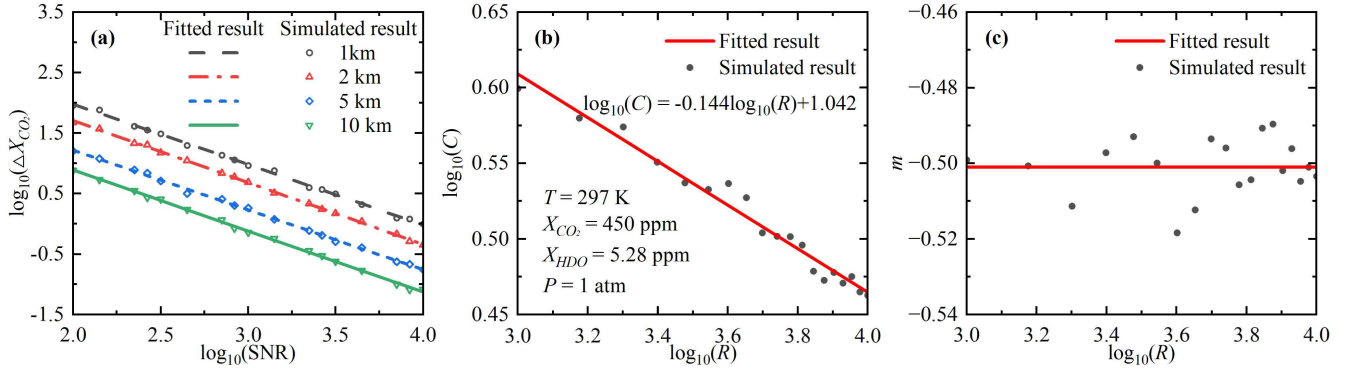


Fig. 12. (a) Relationship between the logarithm of  $X_{CO_2}$ ,  $\log_{10}(\Delta X_{CO_2})$ , and the logarithm of SNR,  $\log_{10}(\text{SNR})$ , at different distances. Dots represent simulation results, while lines show the fitted function  $\log_{10}(\Delta X_{CO_2}) = m \log_{10}(\text{SNR}) + C$ . (b) Relationship between the logarithm of the intercept,  $\log_{10}(C)$ , and the logarithm of  $R$ ,  $\log_{10}(R)$  and (c) relationship between slope  $m$  and the logarithm of  $R$ ,  $\log_{10}(R)$ .

under the conditions of a temperature of 297 K and a  $X_{CO_2}$  of 450 ppm as an example, the results are shown in Fig. 12(a). As shown in the figure,  $\log_{10}(\Delta X_{CO_2})$  decreases monotonically with increasing  $\log_{10}(\text{SNR})$  at different detection distances and can be fitted with a linear function:  $\log_{10}(\Delta X_{CO_2}) = m \log_{10}(\text{SNR}) + C$ , where  $m$  is the slope of the linear curve and  $C$  is the y-intercept. The fitted coefficients of determination ( $R^2$ ) are all greater than 0.98. The relationship between  $\log_{10}(C)$  and  $\log_{10}(R)$  is shown by the black data points in Fig. 12(b). This relationship can be fitted as  $\log_{10}(C) = -0.144 \log_{10}(R) + 1.042$ , as depicted by the red line in Fig. 12(b). The relationship between  $m$  and  $\log_{10}(R)$  is shown in Fig. 12(c). Since  $m$  only varies slightly, ranging from  $-0.49$  to  $-0.51$ , it is taken as the average value of  $-0.502$ . Analyzing the above process provides the relationships of  $\Delta X_{CO_2}$ ,  $\Delta X_{HDO}$ , and  $\Delta T$  with SNR and  $R$ . In the case of a temperature of 250 K and a CO<sub>2</sub> concentration of 350 ppm, the relationships of  $\Delta X_{CO_2}$ ,  $\Delta X_{HDO}$ , and  $\Delta T$  with SNR and  $R$  can be expressed as

$$\begin{aligned}\Delta X_{CO_2} &= \text{SNR}^{-0.9980} \cdot 10^{R^{-0.1528} \cdot 10^{1.0469}} \\ \Delta T &= \text{SNR}^{-0.9972} \cdot 10^{R^{-0.1727} \cdot 10^{1.0739}} \\ \Delta X_{HDO} &= \text{SNR}^{-0.9994} \cdot 10^{R^{-0.3624} \cdot 10^{1.4728}}\end{aligned}\quad (22)$$

In the case of a temperature of 297 K and a CO<sub>2</sub> concentration of 450 ppm, the expressions can be updated as follows:

$$\Delta X_{CO_2} = \text{SNR}^{-1.0020} \cdot 10^{R^{-0.1442} \cdot 10^{1.0417}}$$

$$\begin{aligned}\Delta T &= \text{SNR}^{-1.0000} \cdot 10^{R^{-0.1676} \cdot 10^{1.0705}} \\ \Delta X_{HDO} &= \text{SNR}^{-1.0076} \cdot 10^{R^{-0.3245} \cdot 10^{1.3730}}\end{aligned}\quad (23)$$

In the case of a temperature of 300 K and a CO<sub>2</sub> concentration of 550 ppm, the expressions can be updated as follows:

$$\begin{aligned}\Delta X_{CO_2} &= \text{SNR}^{-0.9978} \cdot 10^{R^{-0.1533} \cdot 10^{1.0735}} \\ \Delta T &= \text{SNR}^{-0.9962} \cdot 10^{R^{-0.1838} \cdot 10^{1.1140}} \\ \Delta X_{HDO} &= \text{SNR}^{-0.9968} \cdot 10^{R^{-0.3646} \cdot 10^{1.4984}}\end{aligned}\quad (24)$$

Under atmospheric pressure conditions at an altitude of 3 km, with  $P$  at 70 108 Pa, HDO set to 0 ppm, a temperature of 297 K, and a CO<sub>2</sub> concentration of 450 ppm, the expressions are updated as follows:

$$\begin{aligned}\Delta X_{CO_2} &= \text{SNR}^{-1.0018} \cdot 10^{R^{-0.1419} \cdot 10^{1.0373}} \\ \Delta T &= \text{SNR}^{-1.0018} \cdot 10^{R^{-0.1657} \cdot 10^{1.0623}} \\ \Delta X_{HDO} &= \text{SNR}^{-1.0028} \cdot 10^{R^{-0.3467} \cdot 10^{1.4473}}\end{aligned}\quad (25)$$

From (22) to (25), it can be observed that the relationships between  $\Delta X_{CO_2}$ ,  $\Delta X_{HDO}$ , and  $\Delta T$  with SNR and distance are similar across the three environmental conditions. For instance, with a temperature of 297 K and a CO<sub>2</sub> concentration of 450 ppm, as the SNR increases from  $10^2$  to  $10^4$  and  $R$  changes from 1 to 10 km, the distributions of  $\Delta X_{CO_2}$ ,  $\Delta X_{HDO}$ , and  $\Delta T$ , as described by (19), are illustrated in Fig. 13(a)–(c), respectively. Comparisons between the analytical results and the simulation results are depicted

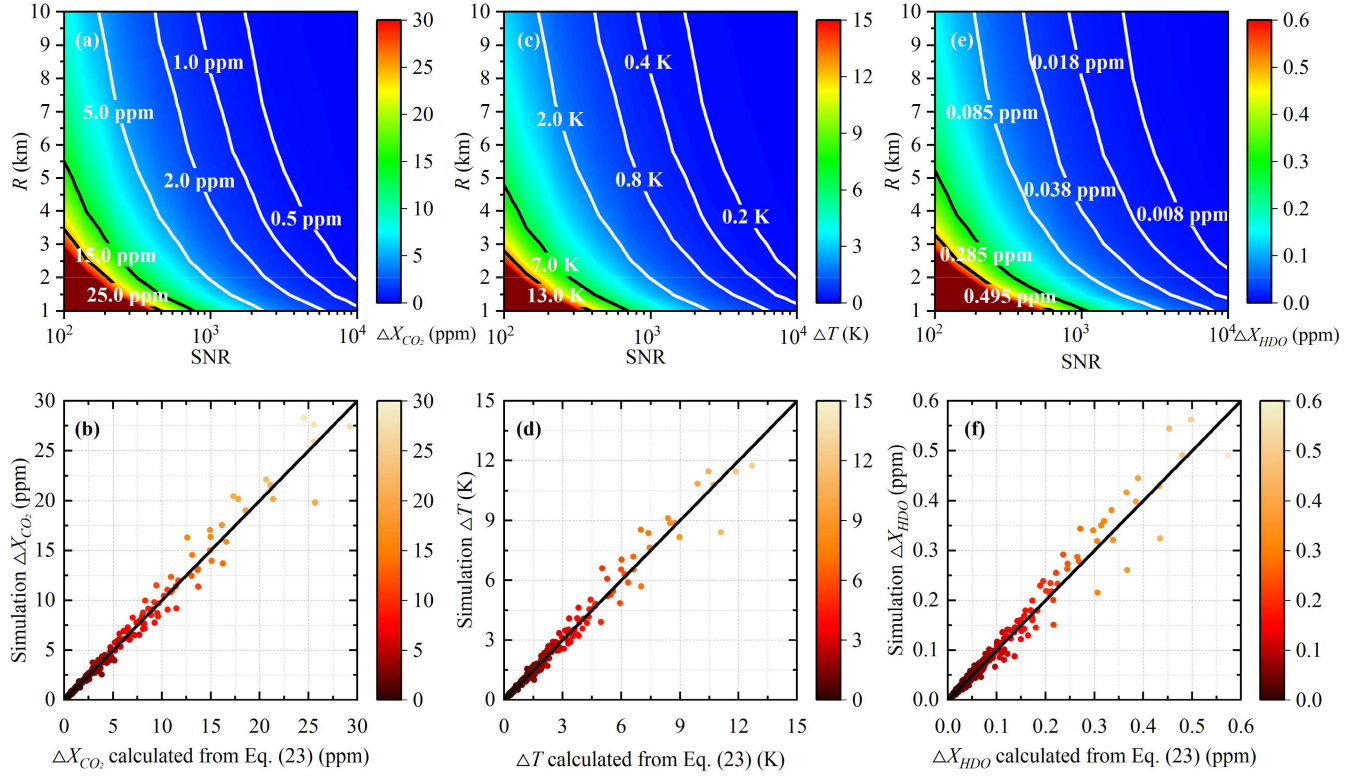


Fig. 13. (a), (c), and (e) Relationship between  $\Delta X_{CO_2}$ ,  $\Delta X_{HDO}$ , and  $\Delta T$  with SNR and  $R$ , respectively, as described by (23). (b), (d), and (f) Comparison between the analytical results, as described by (23), and the simulation results.

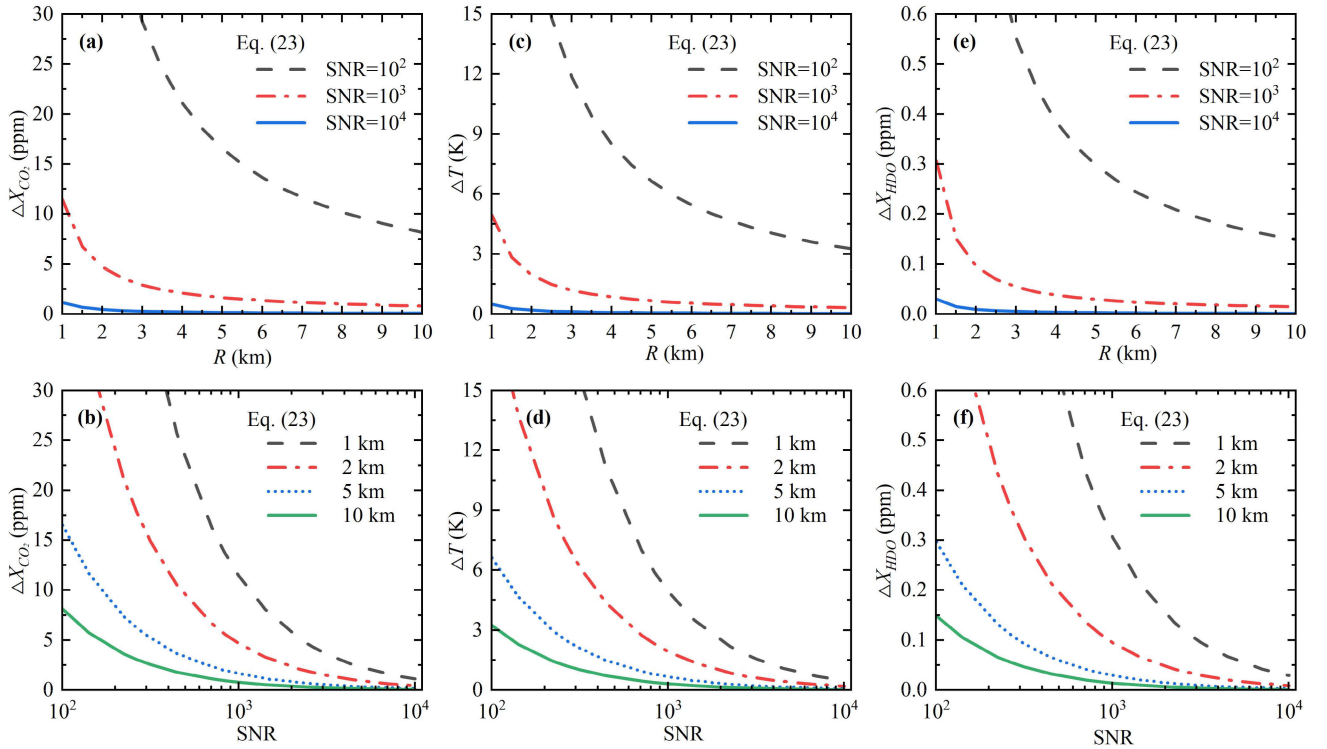


Fig. 14. (a), (c), and (e) Relationship between  $\Delta X_{CO_2}$ ,  $\Delta X_{HDO}$ , and  $\Delta T$  with  $R$ , calculated using (23), under different SNR levels. (b), (d), and (f) Relationship between  $\Delta X_{CO_2}$ ,  $\Delta X_{HDO}$ , and  $\Delta T$  with SNR, calculated using (23), at different  $R$  values.

in Fig. 13(d)–(f). These results demonstrate that the analytical expressions provided by (22)–(25) closely match the simulation results for  $\Delta X_{CO_2}$ ,  $\Delta X_{HDO}$ , and  $\Delta T$ . This indicates that the equations effectively represent the distributions of

TABLE II  
DEFINITIONS AND UNITS OF DIFFERENT SYMBOLS

Parameter	Meaning	Units
$N_S$	The number of photons returned	
$x_i$	Wavenumber (The lidar equation, 30 selected points or DIAL selected points)	$\text{cm}^{-1}$
$x_c$	Central wavenumber of Lorentzian line shape in environmental conditions	$\text{cm}^{-1}$
$R$	Distance	m
$h$	Planck's constant	$\text{kg}\cdot\text{m}^2/\text{s}$
$k_b$	Boltzmann constant	$\text{J}\cdot\text{K}^{-1}$
$T_r$	Transmission term	
$\alpha$	Absorption coefficient of the gas under investigation	$\text{m}^{-1}$
$\alpha_i$	Absorption coefficient of the gas under investigation at the wavenumber of $x_i$	$\text{m}^{-1}$
$OD$	Optical depth	
$UOD$	Unit optical depth	$\text{m}^{-1}$
$N_{\text{CO}_2}$	Molecular number density of CO <sub>2</sub>	molecule / $\text{m}^3$
$X$	Concentration of target gas in the atmosphere	
$X_{\text{CO}_2}$	CO <sub>2</sub> concentration	ppm
$X_{\text{HDO}}$	HDO concentration	ppm
$T$	Ambient temperature	K
$T_0$	Standard atmospheric temperature, 296 K	K
$P$	Ambient pressure	Pa
$P_0$	Standard atmospheric pressure, 101,325	Pa
$w$	Weighting function	
$k$	Fitting slope	
$\Delta T$	Temperature deviation	K
$\Delta X_{\text{CO}_2}$	Error between the CO <sub>2</sub> retrieving results and the CO <sub>2</sub> concentration in the environment	ppm
$B$	Background value of three-peak Lorentz fitting	$\text{m}^{-1}$
$A$	Area of Lorentzian line shape	
$S(T)$	Spectral line intensity at $T$	$\text{cm}/\text{molecule}$
$S(T_0)$	Spectral line intensity at $T_0$	$\text{cm}/\text{molecule}$
$P_{\text{self}}$	Target gas partial pressure	Pa
$\omega_L(P, T)$	Lorentzian HWHM in environmental conditions	$\text{cm}^{-1}$
$n_{\text{air}}$	Coefficient of the temperature dependence of $\omega_L(P, T)$	
$\gamma_{\text{air}}$	Air-broadened HWHM at $T_0$ and $P_0$	$\text{cm}^{-1}/\text{atm}$
$\gamma_{\text{self}}$	Self-broadened HWHM at $T_0$ and $P_0$	$\text{cm}^{-1}/\text{atm}$
$Q(T_0)$	Total internal partition sum at $T_0$	

$\Delta X_{\text{CO}_2}$ ,  $\Delta X_{\text{HDO}}$ , and  $\Delta T$  under varying SNR and distance conditions.

TABLE II  
(Continued.) DEFINITIONS AND UNITS OF DIFFERENT SYMBOLS

$Q(T)$	Total internal partition sum at $T$	
$c_2$	Second radiation constant	$\text{cm}\cdot\text{K}$
$x_0$	Wavenumber of the spectral line transition in vacuum	$\text{cm}^{-1}$
$E''$	Lower-state energy	$\text{cm}^{-1}$
$P_{\text{shift}}$	Pressure shift at the spectral line position	$\text{cm}^{-1}/\text{atm}$
$\text{abundance}$	Abundance of target isotope in nature	

To illustrate these relationships more intuitively, Fig. 14(a)–(c), respectively, shows  $\Delta X_{\text{CO}_2}$ ,  $\Delta X_{\text{HDO}}$ , and  $\Delta T$  variations with the detection range  $R$ , at different SNR levels. Additionally, Fig. 14(d)–(f) demonstrates  $\Delta X_{\text{CO}_2}$ ,  $\Delta X_{\text{HDO}}$ , and  $\Delta T$  variations with the SNR at different distances  $R$ . From Fig. 14, it can be observed that when the SNR is fixed,  $\Delta X_{\text{CO}_2}$ ,  $\Delta X_{\text{HDO}}$ , and  $\Delta T$  decrease as the distance  $R$  increases. Similarly, when  $R$  is fixed,  $\Delta X_{\text{CO}_2}$ ,  $\Delta X_{\text{HDO}}$ , and  $\Delta T$  decrease as the SNR increases. From Fig. 14(a), (c), and (e), when the SNR is  $10^4$ , the distance is between 1 and 10 km,  $\Delta X_{\text{CO}_2}$  is less than 1.5 ppm,  $\Delta T$  is less than 1 K, and  $\Delta X_{\text{HDO}}$  is less than 0.04 ppm. For convenience, the definitions and units of the symbols used in this article are listed in Table II.

## VII. CONCLUSION

This work proposes an algorithm for simultaneously measuring column-averaged atmospheric CO<sub>2</sub>, temperature, and HDO using absorption spectrum lidar, validated through simulations. To reduce system errors, the absorption spectrum was decomposed, and a new model with five Lorentzian peaks and a polynomial background was introduced. The number of fitting parameters was reduced from 18 to 5 through theoretical calculations, significantly decreasing fitted errors. Additionally, simulations established analytical solutions for CO<sub>2</sub>, temperature, and HDO under different SNR and detection distances, considering photon counts that follow shot noise (i.e., single-photon detection), thus validating the method's effectiveness. In future work, single-photon CO<sub>2</sub> absorption spectrum lidar experiments will be conducted to validate the practicality of this approach. Furthermore, the measurement capability will be extended from the current column concentrations to distance-resolved measurements. Finally, this technology, combined with wind speed detection capabilities, is expected to be used for eddy covariance measurements of ecosystem CO<sub>2</sub> flux and industrial pollution monitoring applications.

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