

On-orbit Wavelength Calibration Error Analysis of the Spaceborne Hyperspectral Greenhouse Gas Monitoring Instrument Using the Solar Fraunhofer Lines

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Abstract: Accurate on-orbit wavelength calibration of spaceborne hyperspectral payload is the key to quantitative analysis and application of observational data. Due to the high spectral resolution of the general spaceborne hyperspectral greenhouse gas (GHG) detection instruments, the common Fraunhofer lines in the solar atmosphere can be used as a reference for on-orbit wavelength calibration. Based on the performances of a GHG detection instrument under development, this study analyzes the main sources of errors in the on-orbit wavelength calibration method of the instrument using the solar Fraunhofer lines, including the Doppler shift correction error, the instrumental measurement error, and the peak-seek algorithm error. The calibration accuracy was independently calculated for 65 Fraunhofer lines within the spectral range of the instrument. The results show that the wavelength calibration accuracy is mainly affected by the asymmetry of the Fraunhofer lines and the random error associated with instrument measurement, and it can cause calibration errors of more than 1/10 of the spectral resolution at maximum. 49 Fraunhofer lines that meet the requirement of calibration accuracy have been screened at the design parameters of the instrument, which provides a basis and reference for the general hyperspectral GHG detection payload to utilize the solar Fraunhofer line for high-precision on-orbit wavelength calibration.

Keywords: on-orbit wavelength calibration; solar Fraunhofer lines; high-resolution; greenhouse gas

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1. Introduction

In recent years, the global climate problem caused by excessive emissions of CO₂ and other greenhouse gases has gotten more and more serious and has become a global issue of concern to all countries in the world [1–4]. Detecting the distribution of atmospheric CO₂ concentrations is important for understanding global greenhouse gas emissions and uptake and improving understanding of climate change. Spaceborne hyperspectral GHG detection instruments can acquire fine spectral information on surface targets or atmospheric molecules and detect the narrow-band absorption lines of gas molecules in the atmosphere. The GHG concentrations can be inverted based on the depth of the gas absorption spectra. Hyperspectral remote sensing has unrivaled advantages in the inversion of atmospheric composition [5–7]. In 2019, the IPCC explicitly proposed to expand the observation network by adding satellite remote sensing observations and to support and validate the emission inventories through "top-down" flux calculations centered on assimilation models [8]. SCIAMACHY on ESA's Envisat is the world's first atmospheric tropospheric and stratospheric GHG space probe payload [9]. The main satellites dedicated to GHG detection currently in orbit include NASA's OCO-2, JAXA's GOSAT series, Canada's GHGSat, and China's TanSat [10–14]. In addition, several Integrated Earth

Observation Satellites also carry GHG detection payloads, such as ESA's Sentinel-5P, and China's FY-3D and GF-5 satellites [15–17].

For atmospheric hyperspectral remote sensing payloads, the radiometric and spectral calibration accuracy of the measured data is an important factor affecting the inversion of atmospheric composition [18]. Among them, spectral calibration accuracy mainly includes spectral resolution calibration accuracy and wavelength calibration accuracy, which not only directly affects the positioning accuracy of atmospheric absorption spectral lines, but also impacts the radiometric calibration and correction, thus affecting the accuracy of measured radiance. To improve the reliability of quantitative spectral data measured by the hyperspectral GHG detection instruments, we need to perform accurate spectral calibrations in the laboratory to derive the relevant calibration coefficients. However, due to vibration, changes in environmental factors, aging of instrument components, and other factors, changes in detector center wavelength position and spectral resolution will occur after the instrument is operated in orbit with the satellite, so it is necessary to carry out on-orbit spectral calibration of the instruments to calibrate the results of laboratory calibrations [19,20].

On-orbit spectral calibration of hyperspectral remote sensing loads is mainly carried out using characteristic spectral lines with known wavelengths which are generally generated by the internal calibration light source of the payload or by an external light source. At present, one way of on-orbit spectral calibration is to assemble standard lamps with standard emission lines and determine the wavelength shift of the instrument by the change of the emission lines' position. Another way is to add a standard filter with a known absorption line to the optical path and measure the change in absorption line position to achieve calibration. Both of the above methods have certain limitations. The first method requires power consumption to ignite the lamps, and in order to realize the calibration of different bands of the instrument, it is necessary to use a variety of standard lamps covering different wavelength ranges and a rotating mechanism to convert the lamps. The second method also requires a rotating mechanism to move filters in and out of the optical path [21–25]. Both methods increase the demand for satellite resources and require high precision of the rotating mechanism, which reduces the reliability of the calibration.

Spaceborne hyperspectral GHG detection instruments have a high spectral resolution and are capable of resolving the Fraunhofer lines in the solar spectrum, which are caused by the presence of elements in the sun. The Fraunhofer lines are fixed in the solar spectrum and are not affected by absorption in the Earth's atmosphere. They are sharper and the wavelength positions of the absorption peaks are more precise than the Earth observation spectra. This method utilizes the sun's intrinsic characteristic spectral lines as the standard, which reduces the influence of the internal mechanical structure of the payload and reduces the demand on satellite resources. Therefore, in recent years, hyperspectral payloads have often utilized solar Fraunhofer lines for on-orbit wavelength calibration [26,27]. The Medium Resolution Imaging Spectrometer (MERIS) on Envisat was configured both for Earth and diffuser observations and acquired data for Fraunhofer spectral calibration [28]. A solar diffuser was mounted on OCO-2, which is used to acquire routine observation of the Sun. The spectroscopic performance has been routinely monitored in orbit using measurements of the positions and shapes [29]. The variations in the center wavelength of the atmospheric carbon dioxide grating spectrometer (ACGS) carried on TanSat were calculated at the locations of the Fraunhofer lines by comparing solar-viewing measurements and a high-resolution solar reference spectrum [30].

The solar Fraunhofer lines vary greatly in strength and distribution, especially in the visible and near-infrared bands [31,32]. At the same time, the Fraunhofer lines observed by the instrument are limited by design parameters such as the spectral resolution and sampling rate. When the spectral resolution and sampling rate are high, the instruments can accurately resolve the stronger Fraunhofer lines, and on-orbit wavelength calibration based on these lines is feasible; however, when the spectral resolution and sampling rate

are limited, the instruments' observation of Fraunhofer lines may be affected by the asymmetry of the lines themselves and the adjacent absorption lines, which in turn affects the accuracy of wavelength calibration. In addition, due to noise signals and uncertainties in the radiometric calibration, some Fraunhofer lines may not be accurately resolved or the peak-peak accuracy may be reduced, which needs to be discriminated and screened. Finally, the Doppler shift correction of measured spectra and the peak-peak algorithm can also cause errors in the process of wavelength calibration. Therefore, it is important to analyze the accuracy of the on-orbit wavelength calibration method using the solar Fraunhofer lines with respect to the design parameters of the hyperspectral GHG detection instrument and to screen the solar Fraunhofer lines in the spectral range of the instrument to meet the calibration accuracy requirements.

In this study, the design parameters and performance of a GHG detection instrument under development, including spectral range, spectral resolution, sampling rate, signal-to-noise ratio (SNR),  are used as references. A generic spaceborne hyperspectral GHG monitoring instrument (GHG Monitor) is defined which detects atmospheric CO₂ concentration by measuring the atmospheric fine spectrum in the O₂ and CO₂ absorption wavebands, and the solar observation spectrum of the instrument is simulated. Seven typical Fraunhofer lines are selected as examples for each of the three bands. The main sources of errors in the wavelength calibration method based on the solar Fraunhofer lines, including the Doppler shift correction error, the instrument measurement systematic error, random error, and the peak-peak algorithm error, are highlighted through the peak-peak by fitting the simulated measured Fraunhofer lines. The effects of instrumental measurement errors due to spectral resolution, SNR, and other design parameters on the calibration accuracy are also analyzed. Finally, the results of the analysis were used to distinguish the 65 Fraunhofer lines within the design spectral range of GHG Monitor, which offers a basis and reference for the selection of Fraunhofer lines used for on-orbit high-precision wavelength calibration of general hyperspectral GHG detection instruments. Meanwhile, this study analyzes the effect of instrument performance on the accuracy of on-orbit wavelength calibration, which is informative for the design of general GHG detection instruments.

2. Materials and Methods

2.1. Instrument Design Parameters

GHG Monitor band setting center wavelength 0.76 μm O₂ absorption band (O₂A), 1.61 μm weak CO₂ absorption band (WCO₂), 2.06 μm strong CO₂ absorption band (SCO₂). The WCO₂ band is sensitive to the change of CO₂ concentration in the atmospheric boundary layer, and the absorption degree of the spectral line is approximately linear with the CO₂ concentration, which is an ideal spectral band for the inversion of near-surface high-precision CO₂ concentration. The SCO₂ band is more sensitive to suspended particles in the atmosphere and can detect clouds, scattering, and changes in atmospheric pressure and humidity caused by suspended particles [18]. The O₂A band can provide accurate surface pressure information, and when combined with the SCO₂ band, the scattering problems caused by clouds and aerosols can be well mitigated, which can effectively improve the inversion accuracy of atmospheric CO₂ concentration [33]. The spectral resolution represents the full width at half maxima (FWHM) of the instrument line shape (ILS). As the spectral resolution of the instrument increases, the sharper the absorption lines in the measured spectrum, the higher the sensitivity to atmospheric CO₂ concentration. However, as the spectral resolution increases, the instrument detects lower radiant energy and puts forward very high requirements for SNR [34,35]. To meet the requirements of the retrieval accuracy of CO₂ concentration, it is necessary to consider the indicators of the instrument comprehensively. The main design parameters of the GHG Monitor are shown in Table 1:

Table 1. Main design parameters of GHG Monitor.

Band	O ₂ A	WCO ₂	SCO ₂
Detection Objective	Aerosol, surface air pressure	CO ₂	CO ₂ , H ₂ O
Wavelength (nm)	757.5~772.5	1595~1625	2040~2080
Spectral Resolution (nm)	0.04	0.08	0.10
Sampling Rate		3	
SNR			
($\text{photon} \cdot \text{s}^{-1} \cdot \text{m}^{-2} \cdot \text{sr}^{-1} \cdot \mu\text{m}^{-1}$)	350:1@3.8*1e19	340:1@1.55*1e19	230:1@8.4*1e18
Dynamic range			
($\text{photon} \cdot \text{s}^{-1} \cdot \text{m}^{-2} \cdot \text{sr}^{-1} \cdot \mu\text{m}^{-1}$)	1.1*1e17~1.4*1e21	5.7*1e16~4.9*1e20	3.1*1e16~1.7*1e20
Spatial Resolution (km)		<3	
Wavelength Calibration Accuracy		<FWHM/10	
Absolute Calibration Accuracy		5%	
Inter-channel Relative Calibration Accuracy		0.2%	

For a hyperspectral remote sensor with N channels, the output of channel i is shown in the following equation:

$$X_i = \int_{-\infty}^{+\infty} \frac{E_\lambda}{d^2\pi} \beta^2 A \rho(\lambda) \tau_\theta(\lambda) \tau_o(\lambda) S_s(\lambda) R_d(\lambda) R_e(\lambda) d\lambda \quad (1)$$

where E_λ is the solar irradiance at wavelength λ ; β is the instantaneous field of view of the system; A is the effective optical area of the system; $\rho(\lambda)$ is the reflectivity of the ground; $\tau_\theta(\lambda)$ is the spectral transmittance of the atmosphere; $\tau_o(\lambda)$ is the optical efficiency of the system; $S_s(\lambda)$ is the transfer function of the dispersion system of the sensors; $R_d(\lambda)$ is the spectral responsivity of the detector; $R_e(\lambda)$ is the spectral responsivity of the electronics system. The spectral response function of the i th channel of the system is expressed as follows:

$$S_i = \tau_o(\lambda) S_s(\lambda) R_d(\lambda) R_e(\lambda) \quad (2)$$

It can usually be characterized by a super-Gaussian function, i.e., the relative spectral response $R(\lambda)$ of each spectral channel can be expressed by Equation (3), and Figure 1 shows super-Gaussian functions of different orders n :

$$R(\lambda) = a \cdot e^{-\left(\left|\frac{\lambda - \lambda_c}{c}\right|\right)^n} \quad (3)$$

where a is the fitting coefficient, λ_c is the sampling center wavelength of each spectral channel, n is the super-Gaussian order, and the spectral resolution is expressed by the following equation:

$$FWHM = 2c \cdot (\ln(2))^{\frac{1}{n}} \quad (4)$$

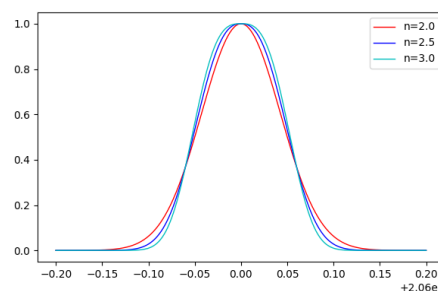


Figure 1. Super-Gaussian functions of different orders n , and the other parameters of the function are as follows: $a = 1$, $\lambda_c = 2060.0$, and $FWHM = 0.1$. When $n = 2$, the function is identical to a general Gaussian.

2.2. Solar Reference Spectrum

In this study, the high-resolution Kurucz solar spectrum is used as the input for the calculation of the simulation spectra of the instrumental solar calibration observations, and it is also used as the reference spectrum for the wavelength calibration method based on the Fraunhofer lines. Its sampling resolution in the O₂A band, WCO₂ band, and SCO₂ band of GHG Monitor is 0.001nm, 0.001nm, and 0.0025nm respectively, and the spectral resolution is one order of magnitude higher than that of GHG Monitor, which meets the requirement of on-orbit wavelength calibration accuracy of the instrument [36,37].

For the calibration method based on the theoretical solar eigen-spectral line, it is first necessary to select the appropriately located Fraunhofer line as the calibration standard. Table 2 and Figure 2 give a total of 21 typical reference Fraunhofer lines in three bands, and the exact positions of the absorption peaks were calculated using the extremum algorithm which regards the positions of the absorption peak minimum as the exact positions of Fraunhofer lines. The Kurucz solar reference spectrum in the SCO₂ band was interpolated to 0.001 nm using the seven-point Lagrange interpolation method.

Table 2. The wavelength position of 21 typical Fraunhofer lines in the three bands.

Band	Fraunhofer lines/nm						
O ₂ A	758.812	761.909	764.238	765.972	767.178	768.239	770.110
WCO ₂	1596.446	1598.513	1600.212	1606.442	1612.039	1613.034	1619.025
SCO ₂	2045.000	2054.431	2056.960	2058.983	2063.533	2070.436	2074.254

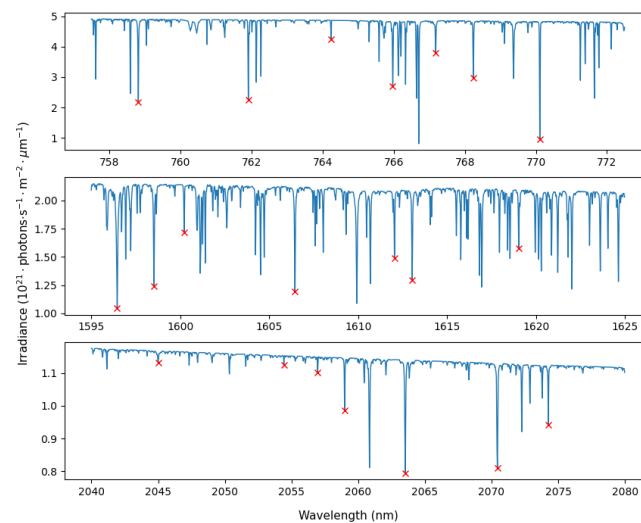


Figure 2. Positions of 21 typical Fraunhofer lines in solar reference irradiance spectra of the three bands, where the positions of Fraunhofer lines are marked by red “x”.

2.3. Simulation of Measurement Spectrum

The simulated instrumental measurement spectrum $I_{simu}(\lambda)$ is obtained by convolving the high-resolution Kurucz solar reference spectrum $I_{ref}(\lambda)$ over the full band at the specified ILS and sampling rate:

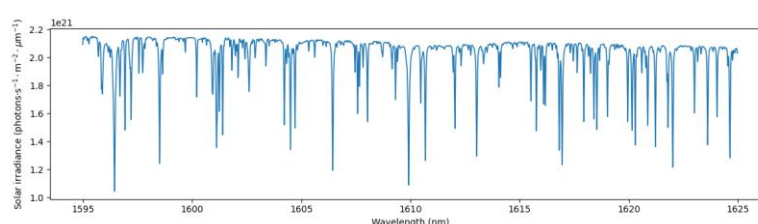
$$I_{simu}(\lambda) = I_{ref}(\lambda) \otimes R(\lambda) \quad (5)$$

Differences in the spectral resolution of each probe element in the band were not considered in this study. The sampling center wavelength λ_c of each spectral channel was calculated using the first-order spectral dispersion equation, i.e.:

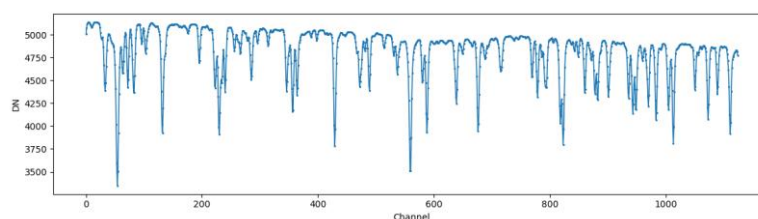
$$\lambda_c = \lambda_0 + column \cdot FWHM / N_{sr} \quad (6)$$

Where λ_0 denotes the starting wavelength of the band, N_{sr} is the sampling rate, and $column$ is the serial number of the spectral dimension probe element.

Considering the instrumental observation parameters, including solar zenith angle, incidence angle, Sun-Earth distance, satellite relative velocity to the sun, diffuser BRDF, A/D quantization efficiency [38], etc., the simulated ideal DN values of the solar observation without considering the dark background signals and noises can be calculated, as shown in Figure 3b. Typical values are used for the instrumental observation parameters, and 14-bit quantization is used for the A/D conversion. By adding the instrument noise signal and radiometric calibration uncertainty, the simulated observation spectral radiance can be calculated. Figure 4 shows the whole simulation process of the instrumental solar measurement spectrum.



(a)



(b)

Figure 3. Simulations of the ideal instrumental solar observation values in the WCO₂ band, where the ILS was simulated using a general Gaussian function with FWHM=0.08nm: (a) the high-resolution Kurucz solar irradiance spectrum in the WCO₂ band; (b) simulated instrumental solar measurement DN values.

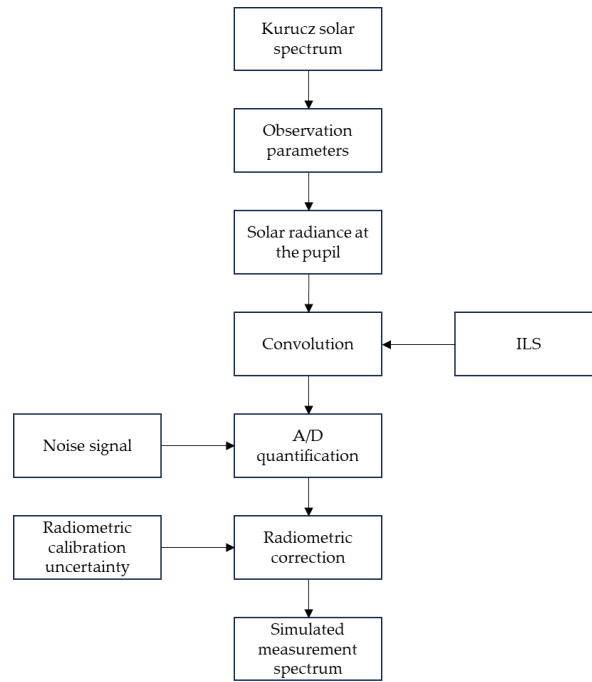


Figure 4. Flow chart of the simulation to calculate instrumental solar measurement spectrum.

For the estimation of instrumental noise, the observation spectra were simulated at the system level in terms of the SNR. The calculation of SNR is carried out in terms of the electron number. The noise electron number N of the system can be considered to be composed of four components, including photon noise $\sqrt{S}$ generated by the input signal, scattering noise $\sqrt{S_{dark}}$ generated by the dark current of the detector, scattering noise $\sqrt{S_{back}}$ generated by the thermal background, and electronic readout noise N_{read} .

$$N = \sqrt{S + S_{dark} + S_{back} + N_{read}^2} \quad (7)$$

S represents the spectral irradiance measured by the detector and can be expressed by the following equation:

$$S = L(\lambda, r, \phi) \times \tau \times QE \times A_{ap} \times \omega \times N_{sr} \times \Delta\lambda \times t_{int} \quad (8)$$

where $L(\lambda, r, \phi)$ is the spectral irradiance detected by the optical system at solar zenith angle ϕ and ground albedo r , τ is the transmittance of the optical system, QE is the quantum efficiency of the detector, A_{ap} is the area of the entry pupil, ω is the instantaneous field-of-view stereo angle of the system, and $\Delta\lambda$ is the spectral bandwidth of the detector's probe element, the value of which is equal to the spectral resolution of the instrument divided by the sampling rate N_{sr} , and t_{int} is the integration time. Equation (9) gives the instrument SNR:

$$SNR = \frac{S}{N} \quad (9)$$

In this study, the SNR at different wavelengths was calculated using the typical spectral irradiance for solar observation of the instrument as input. Ten noise values were calculated for each channel signal based on the SNR combined with the A/D quantization error, and then a random array of numbers was used to add noise to the simulated measurement signals for each channel.

The inter-channel relative radiometric calibration uncertainty is the difference in the consistency of the radiometric calibration of the GHG Monitor across the spectral dimensions of the instrument. For different spectral dimension detectors of the instrument in the same spatial dimension, there is an inconsistency in the radiometric response, which

needs to be corrected in the laboratory and during on-orbit operation [39]. However, due to the existence of uncertainties in the radiometric calibration, there is a certain error in the relative radiometric calibration between spectral channels, i.e., the inconsistency in the radiometric response between spectral channels of the instrument can't be accurately corrected, which leads to uncertainties in the quantitative measurement spectra.

The effect of adding the relative radiometric calibration uncertainty between channels takes the form of adding a percentage uncertainty to the ideal simulated measurement spectra. The radiance of the simulated spectra after adding relative radiometric calibration uncertainty to each channel is given in the following equation:

$$X_{U_i} = X_i \times (1 + P_{uncertainty}) \quad (10)$$

Where X_i is the ideal measured spectral radiance of the i th spectral channel, $P_{uncertainty}$ represents the relative radiometric calibration uncertainty between the channels, which is a random value in the interval $[-\sigma_r, \sigma_r]$, and σ_r is the maximum value of uncertainty.

Figure 5 shows the comparison of the simulated spectrum of the instrumental solar observation in the SCO₂ band before and after adding measurement uncertainty caused by instrumental noise and relative radiometric calibration uncertainty.

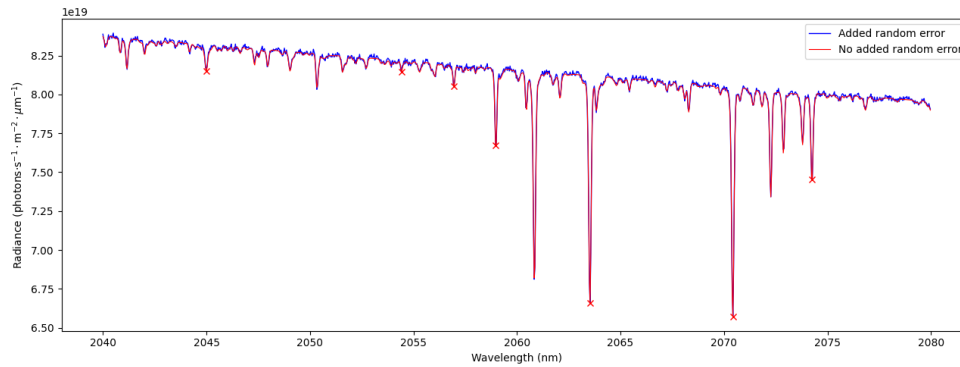


Figure 5. Simulations spectrum of the instrumental solar observation in the SCO₂ band before (red line) and after (blue line) adding measurement uncertainty, where SNR=750:1@8.3*1e¹⁹ photon · s⁻¹ · m⁻² · sr⁻¹ · μm⁻¹ and $\sigma_r=0.2\%$.

2.4. Wavelength Calibration Method

On-orbit wavelength calibration based on the solar Fraunhofer lines determines the position of the absorption peak center by extracting the observed spectra in the vicinity of the Fraunhofer line and using a peak-peek algorithm, typically the Gaussian fitting algorithm. The Gaussian fitting algorithm uses the Gaussian function:

$$y(x) = A \exp\left(\frac{-(x - \mu)^2}{2\sigma^2}\right) \quad (11)$$

to optimally fit the Fraunhofer line of the normalized measurement spectra. It uses the least squares:

$$\sum \text{algorithm}(y(x) - I(x))^2 = \min \quad (12)$$

as the basis of optimization, and the center position of the fitted optimal Gaussian function μ_{opt} as the peak wavelength position, as shown in Figure 6. The wavelength offset is obtained by comparing the fitted peak-peek positions with the positions of the Fraunhofer absorption peaks in the reference spectrum. Figure 7 shows the flow of the on-orbit wavelength calibration method based on the Fraunhofer lines. In the simulation of the measurement spectra in this study, no additional instrumental wavelength offsets were added, so the offset can be regarded as a fixed error for this on-orbit wavelength calibration method under the specific instrumental design parameters.

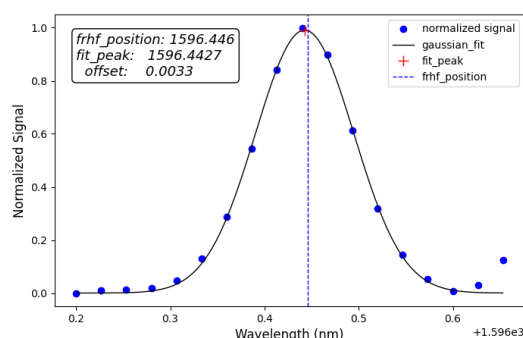


Figure 6. Peak-peek using Gaussian fitting algorithm to the inverted normalized simulated measurement Fraunhofer lines at 1596.446nm in the WCO₂ band: the blue dots represent the inverted normalized simulated measurement values; the black line is the fitted Gaussian function curve; the red “+” is the peak position of fitted Gaussian function curve; blue dashed line marks the actual position of the Fraunhofer absorption peaks in the reference spectrum. The peak-peek position of the measured Fraunhofer line at 1596.446nm is 1596.4427nm, and the offset of peak-peek is 0.0033nm.

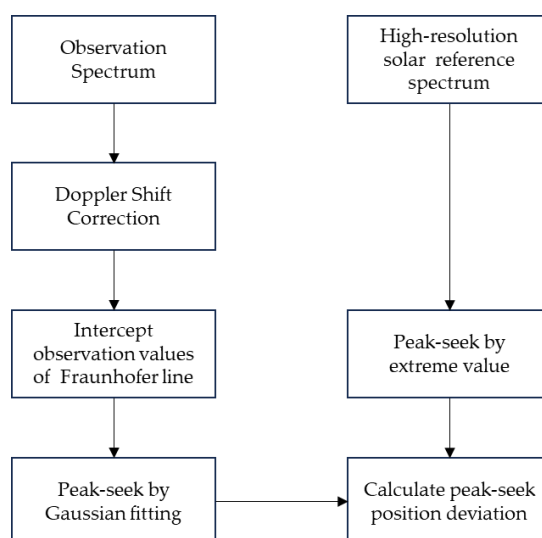


Figure 7. The flow of on-orbit wavelength calibration method based on the solar Fraunhofer lines.

3. Results and Discussions

3.1. Doppler Shift Correction Error

When the instrument is in orbit for solar observation, the relative velocity between the instrument and the sun will produce a wavelength shift, called the Doppler shift which was first discovered and proposed by the Austrian mathematician Doppler. It reflects the relationship between the frequency of the signal and the speed of motion, which is specifically manifested as follows: when the wave source and the receiver are close to each other, the wave is compressed, the wavelength becomes shorter, and the received frequency is greater than the emitted frequency; when the wave source and the receiver are far away from each other, it will produce the opposite effect; the larger the relative speed of motion between the wave source and the receiver, the greater the effect produced.

According to the theory of the Doppler effect, the observed solar spectral frequency increases when the satellite and the sun are close to each other and decreases when they are far away from each other. The Doppler effect can be calculated from the relative velocities of the satellite and the sun, and the revision of the Doppler effect satisfies the following equation:

$$f_d = f(1 + \frac{V_{rel}}{c}) \quad (13)$$

where f_d denotes the Doppler shift, c is the speed of light, and f is the frequency of the original solar irradiance. V_{rel} is the relative velocity of the satellite and the sun, and when V_{rel} is positive, it means that the two are close to each other.

Taking $V_{rel} = 7.0\text{km} \cdot \text{s}^{-1}$ as an example, the wavelength shifts due to the Doppler effect in the three bands are shown in Figure 8. Because of the narrow wavelength range of bands, the wavelength shift due to the Doppler effect at the center wavelength of different spectral channels is very small, which is negligible compared to the spectral resolution of the instrument, and therefore the wavelength shifts of the bands due to the Doppler effect can be analyzed as a whole. The average wavelength shifts of the three bands generated by the Doppler effect are 0.0178 nm, 0.0376 nm, and 0.0476 nm, respectively, which are about FWHM/2 of each band.

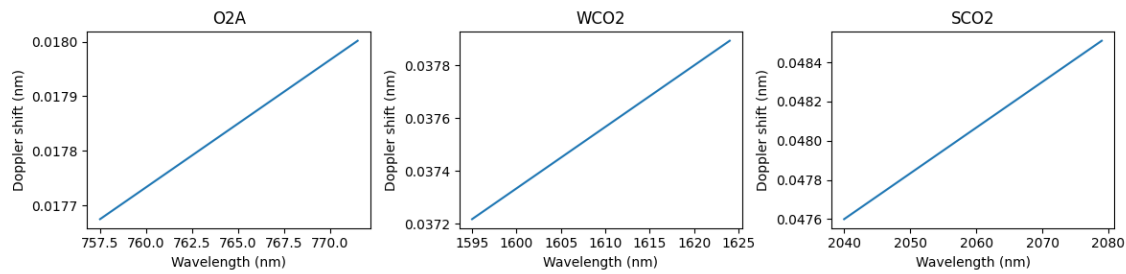


Figure 8. The wavelength shifts at the center wavelength of different spectral channels in the three bands caused by the Doppler effect. The Doppler shifts differences of the starting and ending wavelengths of the three bands are 0.000327 nm, 0.000677 nm, and 0.000910 nm, respectively.

When the instrument is calibrated in orbit, the relative velocity calculation error between the satellite and the sun due to on-orbit timing error, etc., will cause the Doppler shift correction error. From the derivation, it can be seen that δ relative velocity calculation error will cause the same δ Doppler shift correction error, i.e., 2% relative velocity calculation error will cause about FWHM/100 error on the wavelength shift correction. Figure 9 shows the effect of $\pm 5\%$ relative velocity calculation error on the average wavelength shift of the three bands caused by the Doppler effect, using $V_{rel} = 7.0\text{km} \cdot \text{s}^{-1}$ as an example. The average wavelength shift of the three bands caused by a 5% relative velocity calculation error is 0.00089nm,0.00190nm, and 0.00240nm, respectively.

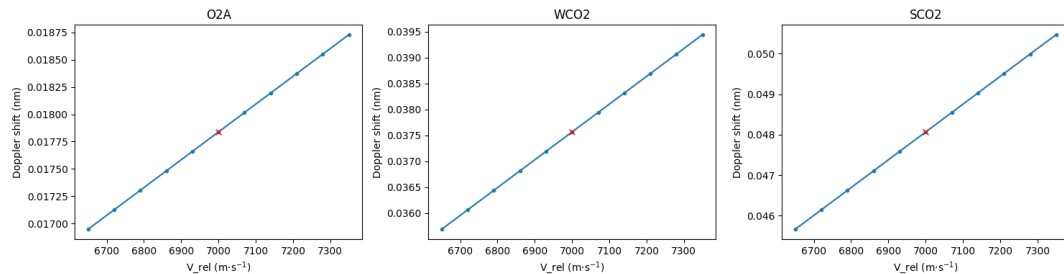


Figure 9. The average Doppler shift correction error of the three bands caused by $\pm 5\%$ relative velocity calculation when $V_{rel} = 7.0\text{km} \cdot \text{s}^{-1}$.

3.2. Systematic Error

When the instrument is loaded and adjusted, the spectral resolution, sampling rate, and ILS of the instrument, and the center wavelength of each spectral channel probe are determined without taking into account the wavelength drift and ILS change. At this time,

due to the spectral broadening caused by the instrumental line function, the observed spectrum obtained after convolution of the solar spectrum near the Fraunhofer line may be affected by the adjacent absorption lines or the asymmetry of the Fraunhofer line themselves, resulting in a deviation between the peak position after convolution and the actual Fraunhofer peak position. This deviation is due to the instrument design parameters, and it's determined under the specified parameters, which can be regarded as the systematic error of this wavelength calibration method. In this case, the peak-peek deviation is mainly caused by the adjacent absorption peaks of the Fraunhofer line and its own asymmetry, and the systematic error is larger for the solar Fraunhofer lines that are more affected by this factor. Taking the positions of the Fraunhofer lines at 1612.039 nm and 1613.034 nm in the WCO₂ band as an example, the convolution spectra of the two absorption lines are shown in Figure 10b. The deviations between the peak positions after peak-peek using Gaussian fitting to the normalized simulated observed spectra and the real solar Fraunhofer peak positions are 0.0115 nm and 0.0004 nm, respectively, as shown in Figure 10c. It can be seen that there is a large deviation due to the effect of the adjacent absorption on the left side of the Fraunhofer line at 1612.039 nm. The relatively symmetrical Fraunhofer line at 1613.034 nm is less affected, which is almost negligible.

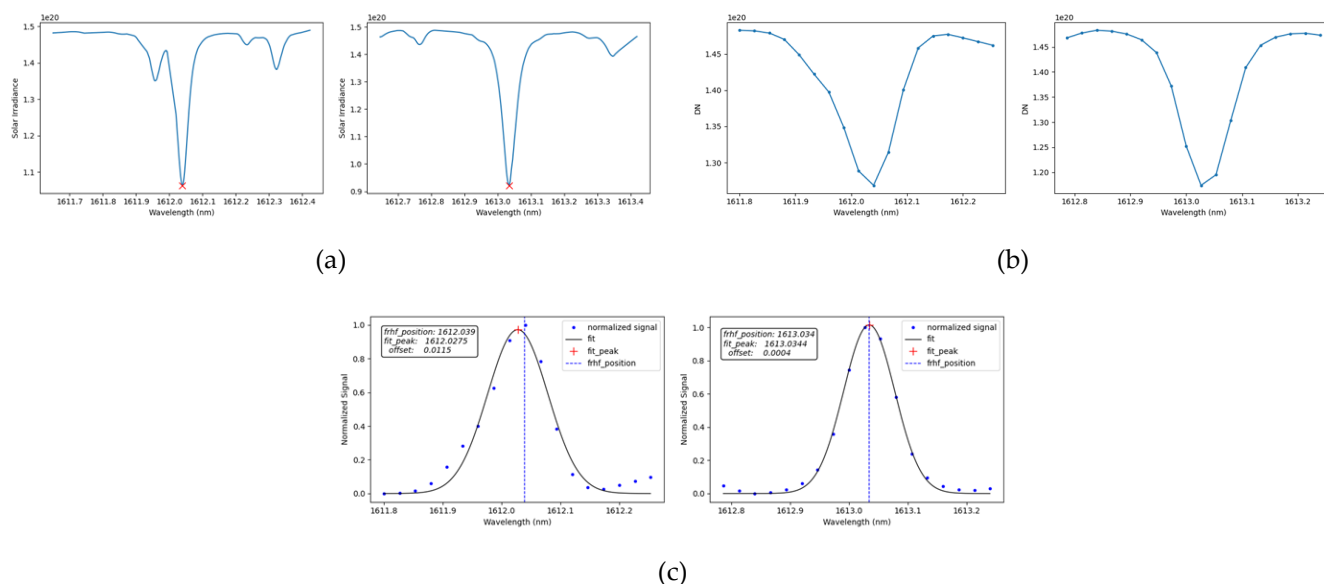


Figure 10. Peak-peek to the simulated measurement Fraunhofer lines at 1612.039 nm and 1613.034 nm in the WCO₂ band: (a) the high-resolution Kurucz solar spectrum at 1612.039 nm and 1613.034 nm; (b) the simulated measurement spectra at the ILS with a general Gaussian function and FWHM=0.08nm; (c) peak-peek using Gaussian fitting algorithm to the normalized simulated measurement Fraunhofer lines.

The center wavelength position of each sampling spectral point can be varied between positive and negative half-wavelength sampling intervals, with which the deviation of the peak-peek position of the observed Fraunhofer line varies. As shown in Figure 11, the systematic error fluctuates around the mean value with the shift of the center wavelength position of each sampling point, but the fluctuation range is small. This result also verifies that the wavelength calibration method based on the solar Fraunhofer line is reasonable under the spectral resolution of the instrument. With the wavelength shift of the sampling point, the deviation of the peak-peek positions of the observed Fraunhofer lines from the positions of the absorption peaks of the solar reference Fraunhofer lines is still affected by the systematic error only, but almost not by the instrumental wavelength shift factor. Therefore, in the actual instrument on-orbit wavelength calibration, after removing the systematic errors, the deviation of the peak-peek position of the Fraunhofer peak can be regarded as the actual wavelength shift of the instrument.

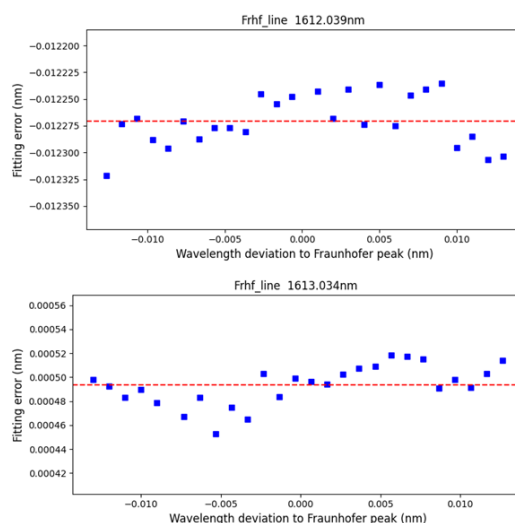


Figure 11. The peak-peek errors (blue dots) of Fraunhofer lines at 1612.039nm and 1613.034nm fluctuate around the mean value (red dashed line) affected by the shift of the center wavelength position of each sampling point.

Increasing the spectral resolution can improve the depiction of the observed spectra, especially the spectra at the absorption peak positions. Therefore, under other conditions, increasing the spectral resolution can enable the instrument to measure the spectra of the absorption peaks of the solar Fraunhofer lines more accurately, thus reducing the systematic error, especially for the more asymmetric lines. The variation of the peak-peek error at 1612.039nm with the spectral resolution is shown in Figure 12. Figure 13 shows the change of the peak-peek systematic error with the increase of the spectral resolution of the instrument. It can be seen that, for the solar Fraunhofer lines with large systematic errors due to strong asymmetry such as 1598.513nm, increasing the spectral resolution has a more obvious reduction effect on the systematic errors, while for the Fraunhofer lines with small systematic errors, the effect is negligible.

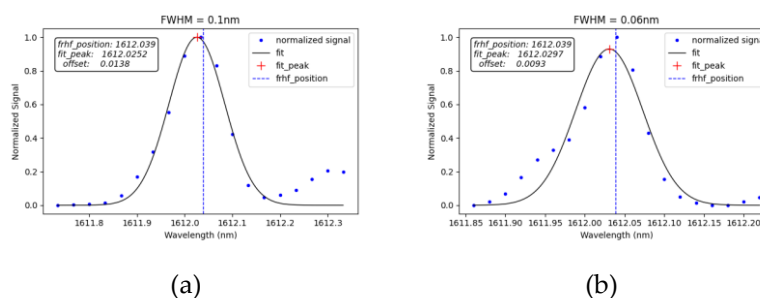


Figure 12. The peak-peek errors at 1612.039nm when (a) FWHM=0.10nm and (b) FWHM=0.06nm. The systematic error caused by the asymmetry of the Fraunhofer line decreases from 0.0138nm to 0.0093nm as the spectral resolution changes from 0.10nm to 0.06nm.

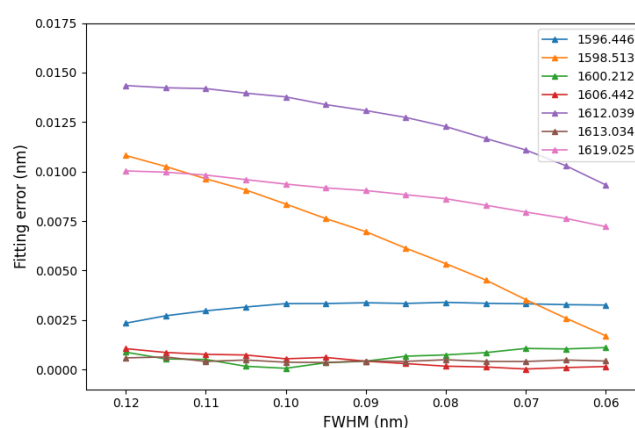


Figure 13. Variation of peak-peak error of the 7 Fraunhofer lines in the WCO₂ band with spectral resolution which changes from 0.06nm to 0.12nm.

The super-Gaussian ILS has a more gentle peak position as the order n increases. As can be seen from the results shown in Figure 14, it has little effect on the peak-peak error of the Fraunhofer lines. In addition, under the condition of certain spectral resolution, the higher the number of sampling points, the smoother and more regular the measured spectral curve is, and the finer the absorption lines characterized by the curve. However, from the analysis, increasing the spectral sampling rate at a certain spectral resolution will not effectively improve the accuracy of the peak-peak position of the Fraunhofer line.

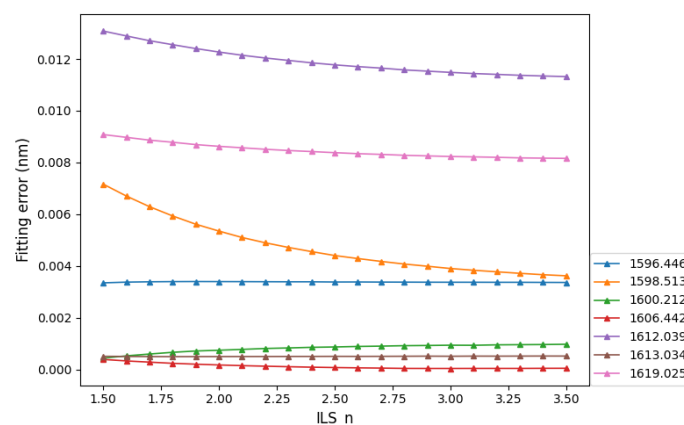


Figure 14. Variation of peak-peak error of the 7 Fraunhofer lines in the WCO₂ band with super-Gaussian function order of ILS which changes from 1.5 to 3.5.

From the above analysis, under the condition of certain spectral resolution, sampling rate, and ILS, due to the asymmetry of the Fraunhofer lines and the influence of the adjacent absorption lines, after the instrumental measurement, the position of the peak-peak using the Gaussian fitting algorithm will have a fixed deviation from the actual solar Fraunhofer peak position. This error can be significantly reduced with the enhancement of the spectral resolution of the instrument but with the super-Gaussian function order of ILS and sampling point of the center wavelength position shift having less impact. In practice, since the design parameters of the instrument have already been determined when the solar Fraunhofer lines are utilized for on-orbit wavelength calibrations, the Fraunhofer lines that do not satisfy the wavelength calibration accuracy due to asymmetry need to be screened and eliminated. In addition, since the systematic error fluctuates less with the shift of the center wavelength position of each sampling point, the effect of the systematic error can be reduced by removing the average deviation, so as to improve the wavelength calibration accuracy. Figure 15 shows the maximum deviation of the peak-peak positions

of the measured spectra from the actual Fraunhofer peak positions after removing the influence of the average systematic error. It can be seen that the peak-peak position errors of the 21 Fraunhofer lines have been significantly reduced after the average systematic errors are corrected, indicating that the peak-peak errors of each Fraunhofer line in the range of the observed bands vary less with the center wavelength position of the sampling point. In addition, the errors of 1612.039nm and 1619.025nm in the WCO₂ band, which are larger than the wavelength calibration accuracy of FWHM/10, meet the requirements after correction. It can be seen that the screening of better symmetry of the Fraunhofer line, as well as the correction of the systematic error is essential to further improve the wavelength calibration accuracy.

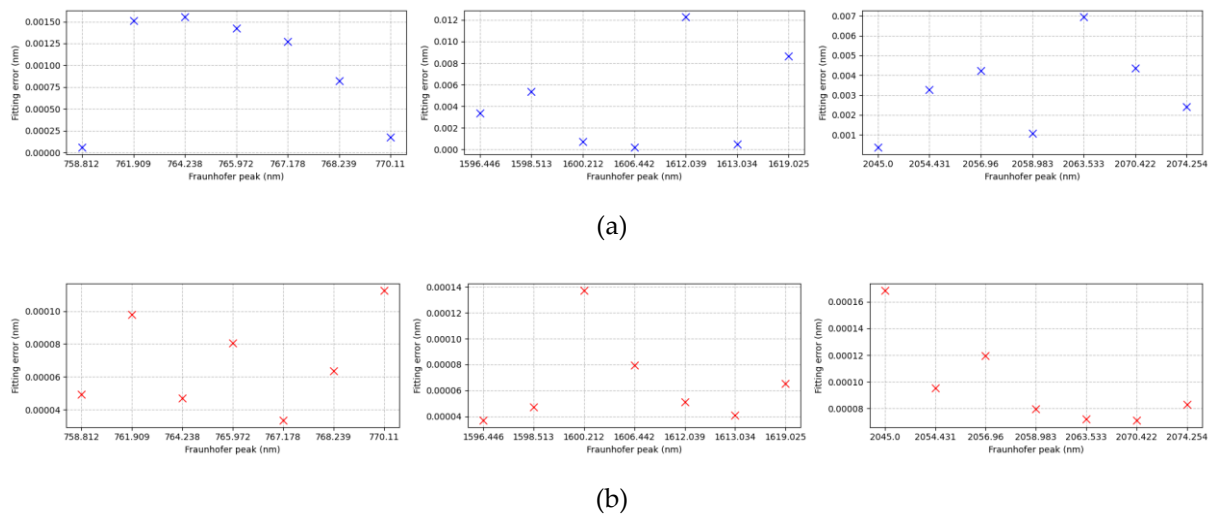


Figure 15. Comparison of the maximum peak-peak errors of the 21 Fraunhofer lines (a) before and (b) after removing the average systematic error in three bands.

3.3. Random Error

In addition to the systematic error associated with the instrument design parameters, the determination of the wavelength position of the observed solar Fraunhofer lines is also affected by random errors due to the noise signal and the uncertainty of the radiometric calibration. The random error mainly has a greater impact on the absorption peaks with weaker intensity. Taking the SCO₂ band as an example, the effects of instrumental SNR and inter-channel relative radiometric calibration uncertainty on the wavelength position seeking of the observed Fraunhofer lines are analyzed.

In order to analyze the effect of observation noise on the wavelength calibration accuracy based on the Fraunhofer lines, the Gaussian fitting of the simulated measurement spectra with the addition of the noise signals is performed to seek the peak at the location of the Fraunhofer lines. Figure 16 shows the peak-peak using Gaussian fitting before and after adding noise at the 2045.0 nm Fraunhofer line, and it can be seen that random fluctuations occur in the observed spectral signals under the influence of noise, which brings uncertainty to the fitted peak-peak position. The experiment was repeated 400 times to statistically measure the effect of the noise signal on the peak-peak error. The peak-peak error is first processed to remove the systematic error before statistics as shown in Figure 17, so that the peak-peak error only characterizes the effect of random error.

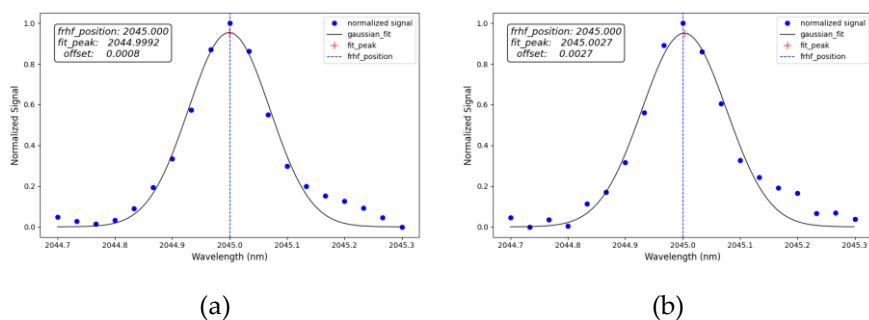


Figure 16. The peak-seeking by Gaussian fitting (a) before and (b) after adding noise at the 2045.000 nm Fraunhofer line. The peak-seeking error increases from 0.0008 nm to 0.0027 nm due to the influence of the noise signal (SNR=750), and thus the random error due to noise is 0.0019 nm.

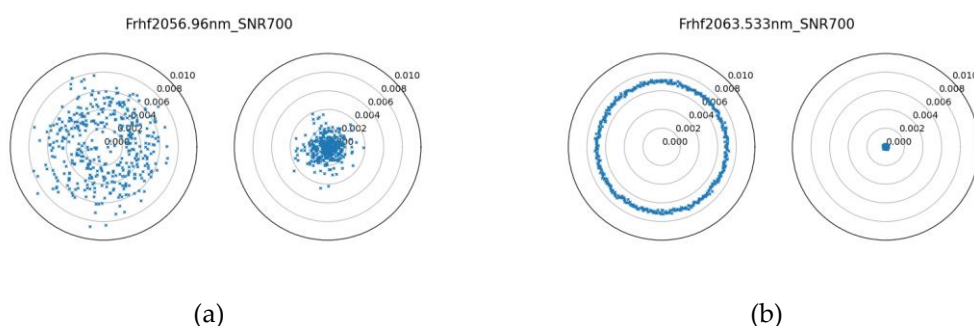
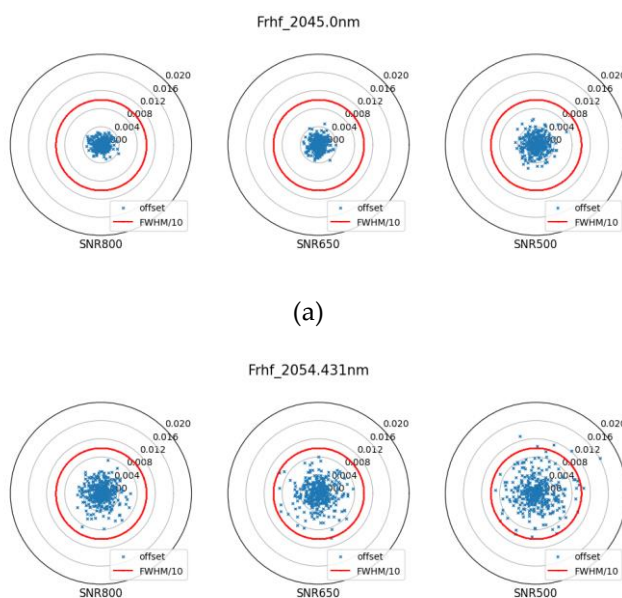


Figure 17. Peak-seeking errors of the Fraunhofer lines at (a) 2056.96 nm and (b) 2063.533 nm before (left figure) and after (right figure) removing the systematic error. The blue data points denote the peak-seeking position error values of 400 experiments.

Calculating the peak-seeking error of each Fraunhofer line in experiments, Figure 18 shows the effect of the peak-seeking error of the three Fraunhofer lines at 2045.0 nm, 2054.431 nm, and 2074.254 nm with the decrease of SNR. It can be seen that as the SNR decreases, the three Fraunhofer lines show a gradual dispersion of the random error, the maximum random error increases, and the weaker the absorption intensity of the Fraunhofer line is affected to a greater extent.



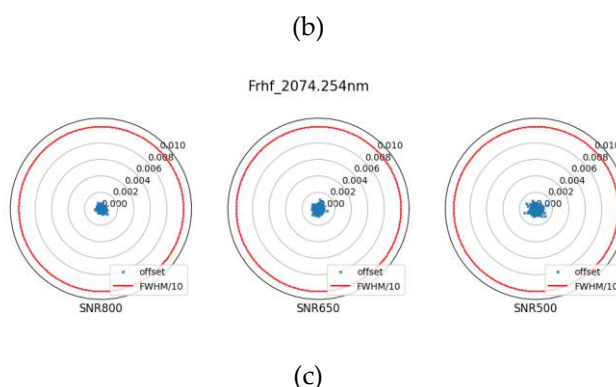


Figure 18. Peak-seeking errors of the Fraunhofer lines at (a)2045.0nm, (b)2054.431nm, and (c)2074.254nm as the SNR is 800, 650, and 500, where the red line is the boundary of FWHM/10.

The variation of the maximum peak-seeking error with SNR for each Fraunhofer line in the SCO₂ band was statistically analyzed. As can be seen from the statistical curve in Figure 19, the maximum random error gradually increases with the decrease of the SNR, especially for the Fraunhofer lines at 2045.0 nm, 2054.431 nm, and 2056.96 nm, which is due to the fact that the peak absorption intensity of the three lines is weaker. The Fraunhofer line at 2054.431nm is most affected by the noise signal, and the phenomenon of fitting peak shift and a large random error occurs when the SNR is higher, so the Fraunhofer line should be considered to be eliminated during wavelength calibration. In addition, the random errors of the peak-seeking at 2045.0 nm and 2056.96 nm when the SNR is lower than 700 exceed FWHM/20, which affects the wavelength calibration accuracy to a certain extent. The other Fraunhofer lines are less affected by the noise signal, and the random error generated by the measurement noise has a negligible effect on the wavelength calibration accuracy.

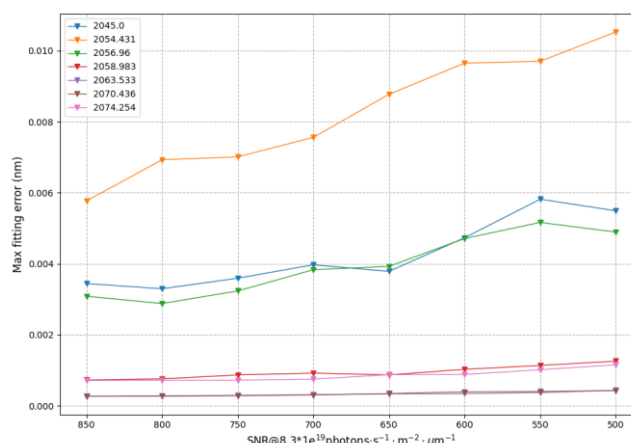


Figure 19. Variation of peak-seeking error of the 7 Fraunhofer lines in the SCO₂ band with SNR which changes from 500 to 850.

The process of analyzing the random errors generated by the radiometric calibration uncertainty is consistent with that used to analyze the effect of the noise signal. Since the radiometric calibration uncertainty affects the observed spectra in a percentage multiplicative form, it has a greater impact than the superimposed form of the noise signal. As shown in Figure 20, for the maximum random error, the Fraunhofer lines at 2045.0nm, 2054.431nm, and 2056.96nm are still larger. Among them, the peak-seeking error of 2054.431nm is too large when the uncertainty is more than 0.1%, and the peak-seeking error of 2045.0nm, 2056.96nm is greater than the FWHM/10 when the uncertainty is more than 0.2%. In practical applications, it's necessary to control inter-channel relative radiometric

calibration accuracy at 0.2% or less to meet the wavelength calibration accuracy requirements or eliminate those Fraunhofer lines that are highly affected by the radiometric calibration uncertainty.

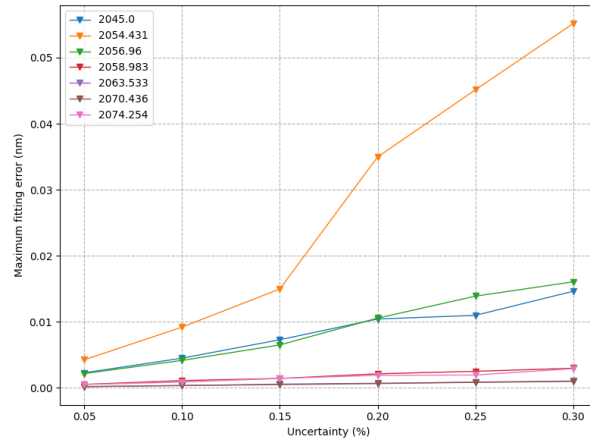


Figure 20. Variation of peak-peak error of the 7 Fraunhofer lines in the SCO₂ band with the inter-channel relative radiometric calibration uncertainty which changes from 0.05% to 0.3%.

For the O₂A and WCO₂ bands, the peak-peak errors are less affected by random errors due to the higher SNR and the high intensity of the Fraunhofer lines. The random error of the peak-peak due to measurement noise and inter-channel relative radiometric calibration uncertainty is less than FWHM/20 for the Fraunhofer lines in both bands. Therefore, the random errors of wavelength calibration using the Fraunhofer lines are negligible for the O₂A and WCO₂ bands.

3.4. Peak-peak Algorithm Error

In addition to the Gaussian fitting algorithm, the center-of-mass algorithm and the cubic spline fitting algorithm are also commonly used for peak wavelength detection in spectral analysis, as shown in Figure 21. The center-of-mass algorithm determines the center wavelength of the measured spectrum by calculating the weighted average of the signals. It is calculated by first multiplying the wavelength value of each spectral data point by the measurement value at its corresponding wavelength, and then adding all the results and dividing them by the sum of the measurement values to obtain the weighted average wavelength, which serves as the peak position of the spectrum. Let λ_i and I_i be the wavelength value and spectral radiance at data point i , respectively, and then the peak wavelength of this spectral signal in the range of data points $i \sim k$ is:

$$\lambda_c = \frac{\sum_{i=0}^k \lambda_i \times I_i}{\sum_{i=0}^k I_i} \quad (14)$$

The cubic spline fitting algorithm approximates the measured spectral signal data in the form of the following equation:

$$f = p \sum_{i=0}^{n-1} w_i (y_i - f(x_i))^2 + (1 - p) \int_{x_0}^{x_{n-1}} \lambda(x) (f^n(x))^2 dx \quad (15)$$

, and then the peak wavelength position of the signal is obtained by utilizing the extreme value peak-peak method for the fitted signal. Where w_i is the i th element of the weights, $\lambda(x)$ is the segmented constant function, and p is the equilibrium parameter, which takes values in the interval $[0,1]$ to make the fitted curves smooth and close to the data points.

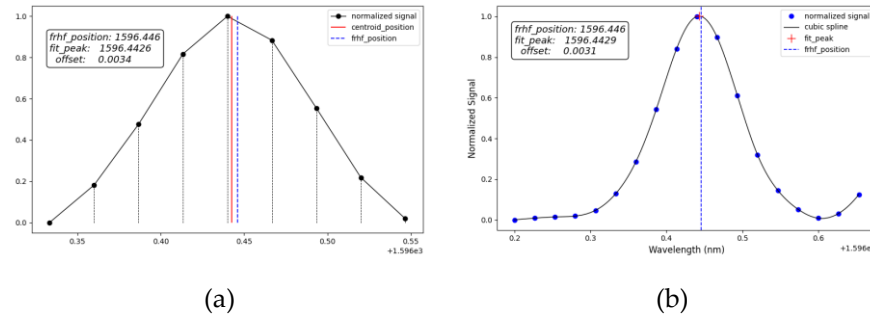


Figure 21. Peak-peek using (a) center-of-mass algorithm and (b) cubic spline fitting algorithm to the normalized simulated measurement Fraunhofer lines at 1596.446 nm in the WCO₂ band.

In order to analyze the influence of peak-peek algorithms on the accuracy of the peak-peek position for the observed solar Fraunhofer lines, three algorithms were used in turn to calculate the peak position and statistically estimate the peak-peek position error. Among them, the center-of-mass algorithm is sensitive to the length of selected sampling points, so 3 times N_{sr} sampling points were intercepted for the calculation. In addition, the length of the selected sampling points will also have a certain degree of influence on the results of the cubic spline function fitting algorithm and the Gaussian fitting algorithm, and 6 times N_{sr} sampling points were intercepted for calculation in this study.

Comparing the results of the three peak-peek algorithms shown in Figure 22, the center-of-mass algorithm is the most sensitive to the asymmetry of the Fraunhofer lines, followed by the Gaussian fitting algorithm, and the cubic spline function fitting algorithm has a higher peak-peek accuracy for the asymmetry Fraunhofer lines. However, compared with the cubic spline fitting algorithm, the Gaussian fitting algorithm is less affected by the central wavelength shift of the sampling point, so the maximum peak-peek error after systematic error correction is smaller than the cubic spline fitting algorithm. As shown in Figure 23, the two Fraunhofer lines at 1612.039 nm and 1613.034 nm are still analyzed, and for the cubic spline fitting peak-peek algorithm, the maximum deviation of peak-peek error due to the central wavelength shift at the two points is 5.9×10^{-4} nm and 5.5×10^{-4} nm, respectively, while for the Gaussian fitting algorithm, the maximum deviation at the two points is 5.1×10^{-5} nm and 4.1×10^{-5} nm. Therefore, in the actual wavelength calibration, the Gaussian fitting algorithm has higher correction accuracy for the wavelength shift of the instrument, but it is necessary to select the absorption lines with a higher degree of asymmetry or to calculate and revise the systematic error.

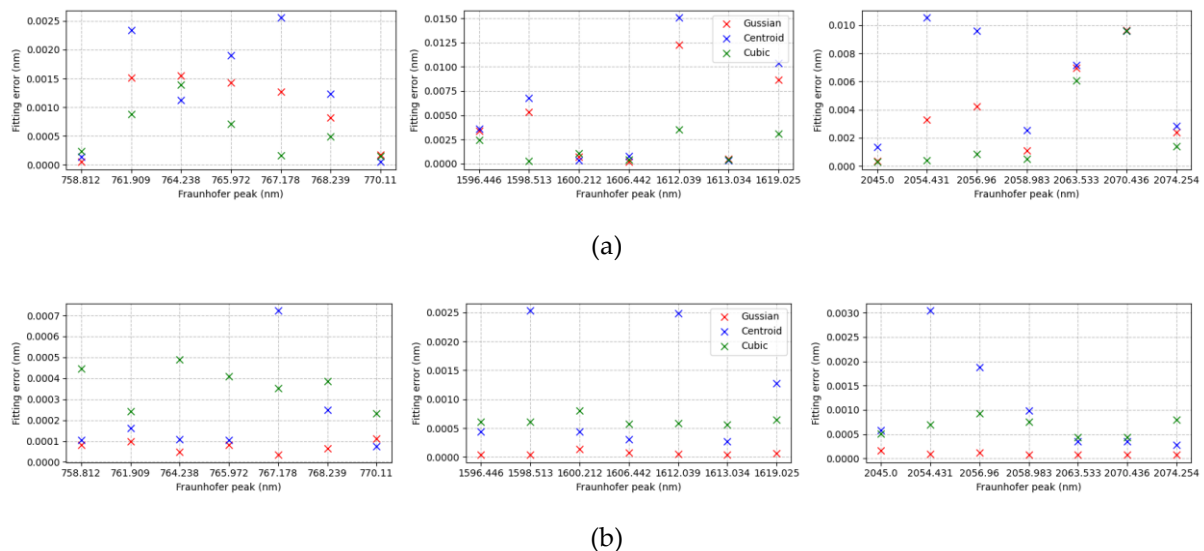


Figure 22. The peak-peak errors of the Fraunhofer lines (a) before and (b) after removing the systematic error in three bands using Gaussian fitting (red “x”), center-of-mass (blue “x”), and cubic spline fitting (green “x”) algorithm.

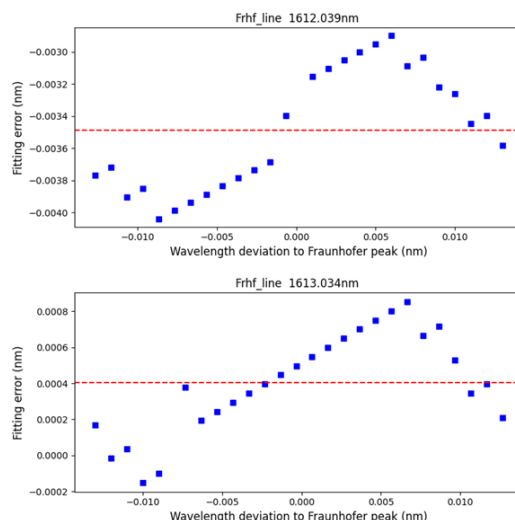


Figure 23. The peak-peak errors of Fraunhofer lines at 1612.039nm and 1613.034nm affected by the shift of the center wavelength position of each sampling point using the cubic spline fitting algorithm. The red dashed line is the reference line of the average value of peak-peak errors (blue dots).

In addition, for the simulated measurement spectra obtained by convolving the ILS in the form of a super-Gaussian function, the peak-peak calculations were also considered by fitting the super-Gaussian function of the corresponding order. For the simulated spectra calculated using the super-Gaussian ILS ($n=2.5$ and $n=3.0$), the Fraunhofer lines in the three bands were fitted with the corresponding order super-Gaussian function, and the results are shown in Figure 24. From the results, it can be seen that the peak-peak using the corresponding super-Gaussian function of ILS does not significantly affect the accuracy of the peak-peak position.

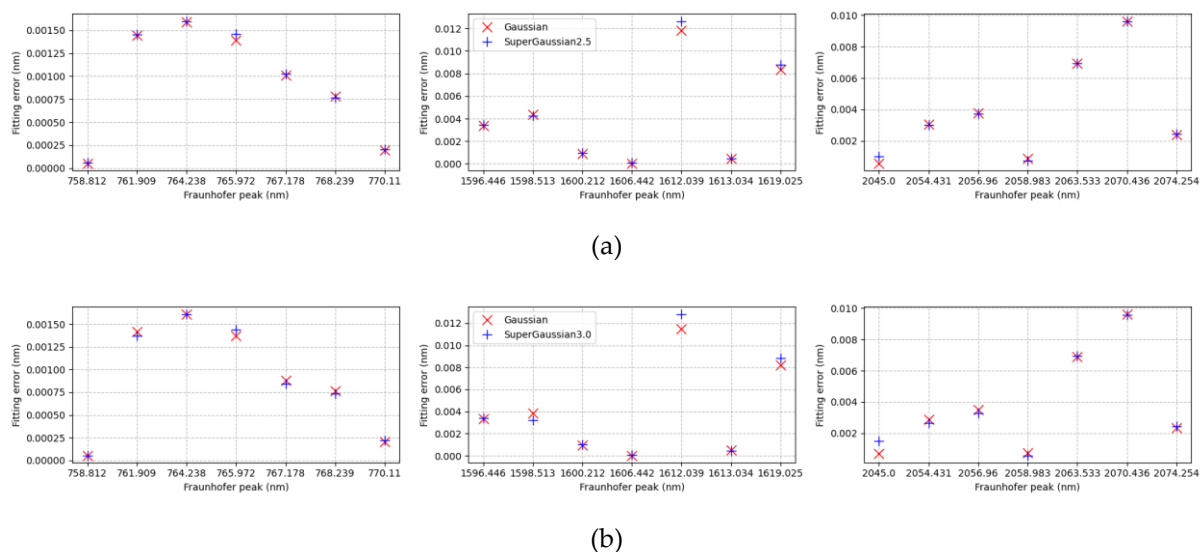


Figure 24. The peak-peak errors of the Fraunhofer lines in three bands using the super-Gaussian function fitting algorithm with the corresponding order of ILS: (a) the order of the super-Gaussian function is 2.5; (b) the order of the super-Gaussian function is 3.0. The peak-peak errors are after removing the systematic error.

3.5. Results of Screening

Using the above analytical method, the wavelength calibration error was calculated for all the solar Fraunhofer lines in the three bands. Firstly, the Fraunhofer lines with small absorption intensity or narrow wavelength width, and the lines greatly affected by the adjacent absorption peaks and their asymmetry were eliminated. The remaining available solar Fraunhofer lines were 21 in the O₂A band, 25 in the WCO₂ band, and 19 in the SCO₂ band. The 65 Fraunhofer lines are distinguished according to the wavelength calibration systematic error, and the results are shown in Figure 25. Among them, 56 lines meet the requirement of FWHM/10 wavelength calibration accuracy, including 46 lines with calibration accuracy less than FWHM/20, and 9 lines need to be corrected for systematic error to meet the calibration accuracy.

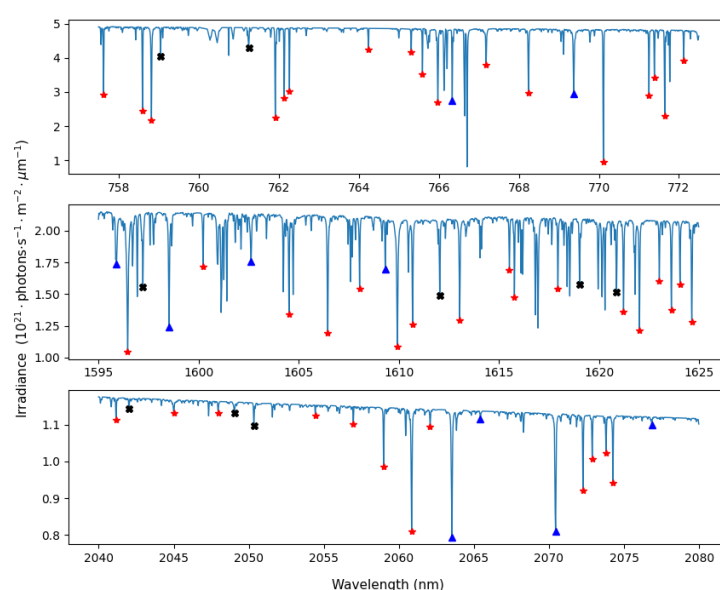


Figure 25. Selection of Fraunhofer lines in the three bands according to the systematic error: the black “X” marks indicate that the peak-peak systematic error of the Fraunhofer line is $>FWHM/10$; the blue “^” marks indicate that the systematic error is $<FWHM/10$ and $>FWHM/20$; the red “*” marks indicate that the systematic error is $<FWHM/20$.

In addition, the random errors of wavelength calibration of 19 Fraunhofer lines in the SCO₂ band were analyzed, as shown in Figure 26, which shows the random errors of peak-peak positions of Fraunhofer lines in the SCO₂ band at SNR=700 and Uncertainty=0.2%. It can be seen that, affected by the random error, the number of Fraunhofer lines in the SCO₂ band that meet the requirements of FWHM/10 wavelength calibration accuracy is reduced to 11, and two of them at 2050.339 nm and 2070.436 nm are subject to systematic error correction.

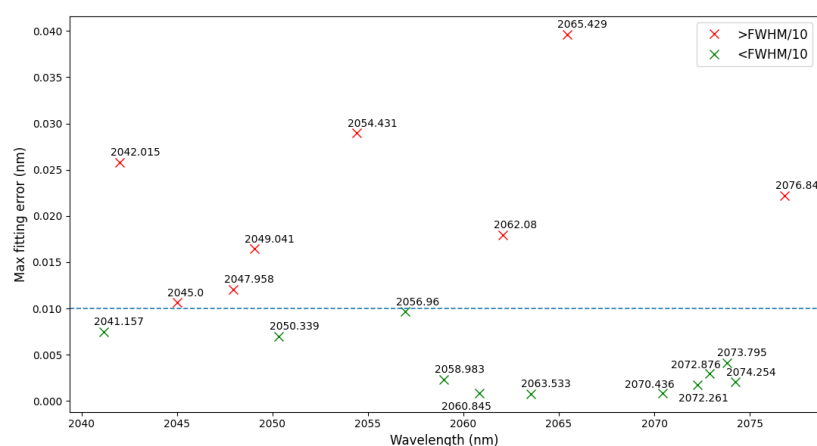


Figure 26. The random errors of peak-peak positions of 19 Fraunhofer lines in the SCO₂ band (SNR=700, Uncertainty=0.2%); the blue dashed line is the reference line of FWHM/10, and the position of Fraunhofer line is marked by green “x” if the random error is less than FWHM/10 while it’s marked by red “x” if the random error is greater than FWHM/10.

4. Conclusion

It is feasible to utilize the solar Fraunhofer lines in the solar observation spectrum for on-orbit wavelength calibration under the design parameters of GHG Monitor, and the accuracy can meet the requirements of less than FWHM/10. The error source of this method is mainly due to the asymmetry of the Fraunhofer lines and the random error of the instrument measurement, which can reach a maximum of more than FWHM/10 and can be reduced by improving the spectral resolution, suppressing the noise of the instrument, and improving the accuracy of the radiometric calibration. The Doppler shift correction error caused by the relative velocity calculation error between the satellite and the sun is limited, and its influence on the wavelength calibration accuracy is less than FWHM/40 under the condition that the relative velocity calculation error is less than 5%, which is almost negligible. About the peak-peak algorithm, the center-of-mass method is the least applicable, and the cubic spline function fitting algorithm has a higher peak-peak accuracy for the asymmetry Fraunhofer lines compared with the Gaussian fitting, but the Gaussian fitting algorithm is less affected by the central wavelength shift of the sampling point.

Under the current parameter design, the number of Fraunhofer lines that can meet the wavelength calibration accuracy of less than FWHM/10 without considering the systematic error reaches 19 in the O₂A band and 21 in the WCO₂ band, which is sufficient for the on-orbit calibration. For the SCO₂ band, some of the Fraunhofer lines are greatly affected by the measurement noise and uncertainty of radiometric calibrations, especially due to the relative radiometric calibration uncertainty between spectral channels. There are 9 directly usable Fraunhofer lines in the SCO₂ band considering measurement uncertainty, and therefore it is necessary to correct accurately the differences in the radiometric responses between different spectral channels in both the laboratory and on-orbit phases.

In practical on-orbit wavelength calibrations of hyperspectral GHG detection instruments, it is necessary to select the Fraunhofer lines with a higher degree of symmetry and absorption intensity in solar-viewing measurement spectra for calibration and conduct a comprehensive analysis of various sources of calibration error in accordance with the on-orbit performance of the instrument. Multi-combined on-orbit calibration modes, including solar observation and Earth observation, should be used in combination to obtain more accurate spectral correction results.

5. Patents

Author Contributions: Conceptualization, C.G. and Y.H.; methodology, Y.G.; formal analysis, Y.G. and F.Z.; resources, C.G. and Y.H.; data curation, Y.G. and F.Z.; writing—original draft preparation, Y.G.; writing—review and editing, Y.G. and Y.L. All authors have read and agreed to the published version of the manuscript.

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Data Availability Statement: The Kurucz solar spectrum used in this study is available at <http://kurucz.harvard.edu/> and other simulation data are contained within the article.

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