Postprint of Research on Wavelength Calibration Method Based on Echelle Grating

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Abstract

Spectral calibration is the prerequisite and foundation for the quantification of instrument remote sensing data. A spectral calibration device based on an echelle diffraction grating was established to address the characteristics of the spaceborne atmospheric trace gas detector, which include a large field of view, wide wavelength range, and high spatial and spectral resolution. The echelle grating operates at high diffraction orders due to its low line density and large blaze angle, offering a wide spectral range and high resolution, and can output multiple relatively uniformly distributed spectral lines within the working band at once, thereby overcoming the shortcomings of traditional calibration methods and improving calibration accuracy. This paper first introduces the working principle of the spectral calibration device, then utilizes this device to perform spectral calibration on the hyperspectral atmospheric trace gas detector, derives the spectral calibration equation for the payload through peak finding and regression analysis, and verifies the calibration results using standard mercury lamp spectral lines. The results show that the pixels and wavelengths of the hyperspectral atmospheric trace gas detector approximately follow a linear distribution, with a calibration uncertainty of 0.0258 nm, and the maximum deviation between the calibrated values and standard values of mercury lamp characteristic spectral lines does not exceed 0.0435 nm, demonstrating the accuracy of the calibration results.

Full Text

Research on Wavelength Calibration Method Based on Echelle Grating

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Abstract

Spectral calibration is the prerequisite and foundation for quantitative remote sensing data analysis. To address the characteristics of a spaceborne atmospheric trace gas detector—namely its large field of view, wide wavelength range, and high spatial and spectral resolution—we have developed a spectral calibration device based on an echelle diffraction grating. Echelle gratings operate at high diffraction orders due to their low groove density and large blaze angle, offering both broad spectral coverage and high resolution. This enables the simultaneous output of multiple uniformly distributed spectral lines within the working band, overcoming the limitations of traditional calibration methods and improving calibration accuracy. This paper first introduces the working principle of the spectral calibration device, then applies it to calibrate a hyperspectral atmospheric trace gas detector. Through peak detection and regression analysis, we derive the instrument' s spectral calibration equation, and finally validate the results using standard mercury lamp spectral lines. The results demonstrate that the detector' s pixels and wavelengths follow an approximately linear distribution, with a calibration uncertainty of 0.0258 nm. The maximum deviation between calibrated and standard values for mercury lamp characteristic lines does not exceed 0.0435 nm, confirming the accuracy of the calibration results.

Keywords: Spectral calibration; Echelle grating; Spaceborne atmospheric trace gas detector; Grating equation

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1. Introduction

To meet the urgent demand for environmental pollution monitoring in China, a hyperspectral atmospheric trace gas detector has been developed for Fengyun satellites. This instrument is a hyperspectral imaging spectrometer based on the Differential Optical Absorption Spectroscopy (DOAS) principle [**?**]. The detector covers a spectral range of 375–500 nm with a total field of view of 112° and a spectral resolution of approximately 0.4–0.6 nm. By detecting atmospheric backscattered radiation from orbit and employing DOAS algorithms, it enables global monitoring of atmospheric trace gas distributions and variations.

Calibration is the prerequisite and foundation for the precise quantitative application of this hyperspectral atmospheric trace gas detector, with spectral calibration being a primary component [**?**]. Spectral calibration determines the spectral characteristics of remote sensing instruments, providing a basis for improving instrument reliability. To ensure high-precision retrieval of trace gas concentrations and their variations, pre-launch spectral calibration of the instrument is essential.

Traditional spectral calibration employs standard spectral lamps [**?**] or tunable lasers [**?**] as light sources. However, spectral lamps provide only a limited number of non-uniformly distributed lines within the instrument' s working range, which significantly impacts the wavelength calibration accuracy for high-resolution spectrometers. Tunable lasers can only calibrate one wavelength at a time, making the calibration of multiple spectral lines for hyperspectral instruments time-consuming and operationally difficult. Furthermore, each scan introduces different errors that affect wavelength calibration precision.

Given the large field of view, wide detection band, and high spatial and spectral resolution of the atmospheric trace gas detector, we have investigated an appropriate spectral calibration method and developed an experimental calibration device based on an echelle diffraction grating. This enables precise full-field spectral calibration of the instrument. We have analyzed the spectral calibration uncertainty and validated the results using mercury lamp spectral lines. Echelle gratings, characterized by low groove density and large blaze angle operating at high diffraction orders, provide broad spectral range and high resolution. The echelle-based calibration device can simultaneously output multiple uniformly distributed high-resolution spectral lines within the 375–500 nm band, overcoming traditional method limitations and improving calibration efficiency and precision. This paper first introduces the working principle of the echelle grating-based calibration device, then performs spectral calibration of the atmospheric trace gas detector, and finally analyzes and evaluates the calibration results.

2.1 Working Principle and Optical Path of the Calibration Device

According to the grating diffraction equation:

$$d(\sin\alpha + \sin\beta) = m\lambda$$

where α is the incident angle, β is the diffraction angle, m is the diffraction order, λ is the central wavelength, and d is the grating constant.

The reciprocal linear dispersion formula is derived as:

$$\frac{d\lambda}{dl} = \frac{10^6 \cos\beta}{mnf}$$

where n is the groove density, dl is the exit slit width, and f is the exit focal length. Transforming equation (2) yields:

$$\Delta\lambda = \frac{10^6 \cos\beta}{mnf} \cdot dl$$

Equation (3) represents the spectral broadening corresponding to the slit width, i.e., the spectral resolution at different wavelengths. To meet the spectral calibration requirements for the atmospheric trace gas detector, the calibration instrument' s spectral resolution should be one-fifth to one-tenth of the instrument under test. The structure of the spectral calibration device is shown in [Figure 1: see original paper] [?].

The echelle grating has 79.01 grooves/mm and a diffraction angle of 71.5°. According to equation (2), when the collimating mirror focal length $f = 615.894$ mm, the spectral resolution of the slit function measurement instrument is 0.0394–0.0578 nm for the 370–505 nm spectral range, satisfying calibration requirements.

The output spectrum of the calibration device is shown in [Figure 2: see original paper]. Table 2 presents the central wavelengths and spectral resolution of the calibration device.

Table 2. Central wavelength and spectral resolution of the equipment

Diffraction order	Central wavelength (nm)	Spectral resolution (nm)

As shown in Table 2, the echelle diffraction grating calibration device can simultaneously output multiple high-resolution spectral lines across 375–500 nm. Leveraging this characteristic for hyperspectral imaging spectrometer calibration ensures accurate spectral line position calculation and enables high-precision spectral calibration.

2.2 Selection of Calibration Light Source

To ensure complete coverage of the 375–500 nm spectral range, the L2479 ultra-quiet xenon lamp from Hamamatsu Photonics is selected as the calibration source. This source features high output power and stable energy distribution. Its primary radiation characteristics are listed in Table 1 .

Table 1. Radiation characteristic of L2479

Power (W)	Arc length (mm)	L2479 intensity (W/cm^2 · nm@50cm) @ =440nm

3. Experimental Process and Results

The spectral lines output by the calibration device were measured using an Andor SR-2234 spectrometer, yielding the spectrum shown in [Figure 2: see original paper]. The central wavelengths and resolution of the output lines are presented in Table 3 .

3.1 Experimental Procedure

The spectral calibration task for the spaceborne atmospheric trace gas detector involves determining the working wavelength corresponding to each pixel, thereby establishing the instrument' s detection band and spectral resolution capability. Due to the instrument's large field of view, spectral curvature occurs. Therefore, to achieve accurate wavelength calibration, the central working wavelength of every pixel across the full field of view must be calibrated, establishing a wavelength distribution matrix in both spectral and spatial dimensions.

The experimental setup is illustrated in [Figure 3: see original paper], consisting of the light source, echelle diffraction grating calibration device, high-precision rotation stage, hyperspectral atmospheric trace gas detector, and computer. After powering on the xenon lamp, measurements begin following a 10-minute stabilization period. Integration time and gain are adjusted to ensure high signal-to-noise ratio. Spectral data from the CCD photosensitive region, denoted as S_{im} and S_{jn}, are recorded, where i and j represent spatial dimension row numbers, and m and n represent spectral dimension column numbers. The rotation stage is turned every 10°, and spectral data S'_{im} and S'_{jn} are recorded. This process is repeated to acquire full field-of-view spectral data.

3.2 Data Processing and Analysis

The spectral calibration process primarily comprises peak detection and least-squares regression. For each spectrum, characteristic spectral lines are first identified through peak detection. Least-squares regression is then applied to correlate wavelengths with pixel numbers, yielding the instrument' s spectral calibration equation. From this equation, the detection channel' s spectral range can be calculated.

After dark count subtraction from the spaceborne atmospheric trace gas detector' s spectral data, several high signal-to-noise ratio spectral lines are selected. Since the Gaussian function well characterizes spectral response, Gaussian fitting is employed for peak detection. The fitting function is given by equation (4):

$$S(X) = A_0 \exp\left(-\frac{(X-x_0)^2}{2\sigma^2}\right)$$

where $S(X)$ represents the instrument count, X is the pixel number, A_0 is the fitting coefficient, x_0 is the pixel number corresponding to the spectral line center, and σ is the full width at half maximum. [Figure 4: see original paper] shows the spectral response curve at 462.46 nm for the central field of view of the atmospheric trace gas detector.

Through fitting, the peak center is determined to correspond to pixel number 490.959, establishing the relationship between this pixel and wavelength 462.46 nm. Peak detection processing yields the correspondence between central wavelengths and pixel numbers. Since spectral lines are approximately linearly arranged on the CCD, least-squares linear regression is applied to the data sets. The regression equations are given by (5) and (6):

$$\begin{cases} \lambda_{im} = aX_{im} + b \\ a = \frac{\sum(X_{im}-\bar{X})(\lambda_{im}-\bar{\lambda})}{\sum(X_{im}-\bar{X})^2} \\ b = \bar{\lambda} - a\bar{X} \end{cases}$$

where i is the row number, m is the column number, λ_{im} is the central wavelength, and X_{im} is the pixel number corresponding to the central wavelength.

[Figure 5: see original paper] shows the regression line for the spaceborne atmospheric trace gas detector in the central field of view. Solid dots represent output wavelengths from the echelle diffraction grating calibration device, while the straight line represents the calibration equation. The calibration equation is given by (7):

$$\lambda_{im} = 0.1716X_{im} + 546.7397$$

with $R^2 = 0.9999$, indicating that wavelength and pixel number approximately satisfy a linear relationship. [Figure 6: see original paper] shows the regression residual plot. The horizontal axis represents the index of points used in regression, and the vertical axis represents residuals. All confidence intervals include zero with no outliers, and the maximum deviation does not exceed 0.04 nm, further confirming the linear relationship between pixel number and wavelength. The detection band calculated from the regression equation is 370–510 nm, meeting the design requirement of 375–500 nm.

3.3 Uncertainty Analysis

The wavelength calibration uncertainty of the spaceborne atmospheric trace gas detector primarily includes calibration source instability, peak detection error, regression analysis uncertainty, and spectral broadening. The output spectral uncertainty of the calibration device depends on the SR-2234 monochromator' s measurement uncertainty, which is 0.01 nm. Peak positioning uncertainty, caused by instrument stability and algorithmic factors, is better than 0.1 pixel.

Regression analysis uncertainty is characterized by residual standard deviation. The error propagation formula is:

$$\sigma = \sqrt{\sigma_1^2 + \sigma_2^2 + \sigma_3^2}$$

where σ is the total wavelength calibration uncertainty of the atmospheric trace gas detector, σ_1 is the output spectral uncertainty of the calibration device, σ_2 is the peak positioning uncertainty, and σ_3 is the regression analysis uncertainty. Using this error propagation formula, the wavelength calibration uncertainty for the central field of view is analyzed in Table 3 .

Table 3. Uncertainty analysis of spectral calibration

Uncertainty source	Value
σ_1 (nm)	
σ_2 (nm)	
σ_3 (nm)	
Total σ (nm)	0.0258

3.4 Verification of Calibration Results

Standard mercury lamp spectral lines are used to verify the wavelength calibration results. Wavelength information is obtained from the calibration equation, and accuracy is validated by comparing calibrated values with standard values for mercury characteristic lines. Table 4 presents the comparison between calibrated and standard wavelengths.

Table 4. The comparison of the calculated value and standard values

Standard wavelength (nm)	Calibrated wavelength (nm)	Absolute deviation (nm)

The comparison results show that the maximum absolute peak deviation does not exceed 0.0435 nm, demonstrating the accuracy of the spectral calibration equation.

4. Conclusion

This paper investigates the spectral calibration technology for a spaceborne atmospheric trace gas detector. Considering the instrument’ s large field of view

and wide detection band, a spectral calibration scheme was established. An ultra-quiet xenon lamp was selected as the calibration source, and an echelle diffraction grating-based spectral calibration device was constructed. The device simultaneously outputs multiple uniformly distributed high-resolution spectral lines across 375–500 nm, improving both calibration efficiency and precision compared with traditional methods. Data processing yielded the spectral calibration equation, which was verified using standard mercury lamp lines. The results show that the relationship between pixel number and wavelength follows the regression line well, with $R^2 = 0.9999$ and a detection range of 370–510 nm, meeting design requirements. Uncertainty analysis yields a calibration uncertainty of 0.0258 nm. This work provides valuable experience for subsequent spectral calibration of spaceborne large-field imaging spectrometers.

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Note: Figure translations are in progress. See original paper for figures.