GOME WAVELENGTH CALIBRATION USING SOLAR AND ATMOSPHERIC SPECTRA

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Abstract

Spectral information in GOME solar irradiance spectra and GOME Earth radiance spectra is used in conjunction with the GOME solar reference spectrum to provide absolute vacuum internal wavelength calibration for GOME. Two methods for wavelength calibration of GOME data are investigated. The first employs chi-square minimization of a merit function involving wavelength and the GOME slit function. It is quite robust and requires little GOME data in the processing (calibration window regions with from 15 to 40 pixels). The second employs cross correlation of GOME data and the solar reference spectrum in the Fourier transform domain, using a procedure in the Image Reduction and Analysis Facility (IRAF; http://iraf.noao.edu) software system developed for the determination of galaxy redshifts. It also requires small amounts of GOME data (calibration window regions with from 10 to 50 pixels). Both methods provide absolute wavelength calibration accurate to a small fraction of a GOME pixel across the entire GOME spectrum, and to 0.001 nm over much of the range.

Keywords Global Ozone Monitoring Experiment; Wavelength calibration; Fraunhofer spectrum

1. INTRODUCTION

GOME derives its primary wavelength calibration from the measurement of positions of lines emitted by a PtNeCr lamp on board the instrument. Lines positions have been shown to be stable to 0.02-0.04 GOME pixel when measured in orbit over a typical range of instrument temperature variation (Hoekstra et al., 1996). The line positions themselves are known to high absolute vacuum wavelength accuracy from a study undertaken expressly for the GOME instrument (Murray, 1994). The wavelength scale is transferred to GOME irradiance and radiance measurements using the temperature at the predisperser prism as a proxy. It has been demonstrated in science studies by members of the GOME Scientific Advisory Group that this transfer can introduce additional uncertainties in the wavelength scale, and that the wavelength coverage of lamp lines is sparse in some of the GOME spectral range. The purpose of the investigations described here is to explore alternative methods of wavelength calibration making use of the spectral structure from solar Fraunhofer lines present in both GOME irradiance and radiance spectra and terrestrial absorption lines present in GOME radiance spectra. Progress to date, as described here, uses chiefly the Fraunhofer lines.

2. SOLAR REFERENCE SPECTRUM CALIBRATION

Both wavelength calibration methods require a solar reference spectrum that itself is well-calibrated in absolute vacuum wavelength. We use the solar reference spectrum developed for GOME (Chance & Spurr, 1996; 1997). This spectrum includes residual terrestrial lines, which are useful both for its own wavelength calibration and for comparison with features in GOME radiance spectra. The reference spectrum wavelength scale for the region 300-800 nm is re-calibrated making use of recently measured positions of O_2 A band lines, including pressure shifts (D. Newnham, J. Ballard & M. Page, private communication, 1997), giving an absolute accuracy of 2 parts in 10^7. This recalibration also applies to the synthetic Ring spectrum that has been developed for GOME and SCIAMACHY applications (Chance & Spurr, 1996; 1997). For wavelengths shortward of 300 nm, the accuracy is currently 0.002 nm; further work is need to improve this.

3. CALIBRATION BY CHI-SQUARE MINIMIZATION

In this method the high resolution solar reference spectrum is degraded to GOME resolution and sampled to the estimated instrument grid. A nonlinear least-squares fitting procedure optimizes the width of the slit function as well as the initial grid spacing in order to minimize the differences between the simulated and GOME spectra.

The calibration is performed for a fixed set of calibration windows in each GOME channel, where each window contains between 15 and 40 detector pixels. Windows are selected visually, looking for regions of the GOME spectrum with "reasonable" levels of structure. This empirical approach selects both strong and well-known Fraunhofer lines and windows with structure contributed by multiple weak lines.

The instrument slit function should be Gaussian, characterized by a standard deviation σ. It is assumed that the pixel spacing within a window remains constant. On-ground calibration data are used to determine an initial guess σ_0 for the slit function and an initial wavelength grid $(\lambda_0, \Delta\lambda_0)$, so that GOME pixel n of the current calibration window has the estimated wavelength $\lambda_0 + n\Delta\lambda_0$.

The shift $d\lambda$, the squeeze factor s, the width of the Gaussian slit function σ, and the quadruplet $(\alpha_0, \alpha_1, \alpha_2, \beta)$ are selected to minimize the merit function:

$$\chi^2 = \sum_i [gome_i - (\alpha_0 + \alpha_1 i + \alpha_2 i^2) \times f(solref, \sigma, \lambda_0 + d\lambda + is\Delta\lambda_0) - \beta]^2$$

where:

- i is the index of a detector pixel within the selected window;
- f is a function that returns the value of the high resolution reference spectrum convolved with a Gaussian kernel of standard deviation σ, at the wavelength specified by its third parameter;
- β accounts for the fluctuations of the dark signal offset; and
- $(\alpha_0, \alpha_1, \alpha_2)$ is a variable scaling factor that takes the variations of the instrument radiance response into account. This permits calibration on raw GOME measurements and is necessary in the overlap regions where the instrument radiometric response is not well known.

The $(\alpha_0, \alpha_1, \alpha_2, \beta)$ are obtained by linear least-squares fitting, whereas the determination of $(d\lambda, s, \sigma)$ requires a nonlinear fitting technique. The Levenberg-Marquardt method is used (Marquardt, 1963).

After optimization, the wavelength of pixel 0 of the calibration window is given by $\lambda_0 + d\lambda$. The algorithm also provides an estimate of the pixel spacing within the window, $s \cdot \Delta\lambda_0$. This information can be used to improve the determination of the fitted calibration curve over the entire channel, especially at the edges where extrapolation is necessary. The estimated slit width is a useful parameter for instrument monitoring, and can be used for further level 1-2 processing when reference data sets (*e.g.*, cross sections) need to be convolved to the GOME resolution.

Figure 1 shows fitting results performed on a solar spectrum acquired on June 28, 1996 and simply corrected for dark signal. The left-hand plots correspond to the first window of channel 1; they show that good fitting quality is obtained even in the UV regions where the light flux is low. The right-hand plots correspond to window 6 of channel 3. They demonstrate the possibility for calibration in a region of the spectrum that contains many small lines.

Figure 2 shows the absolute wavelength calibration uncertainties (1σ) over the entire GOME wavelength range. For most windows the uncertainty is well below 1/50 of a pixel. The degradation of the results in channel 4 may partly be explained by remaining atmospheric features in the solar reference spectrum.

Figure 3 shows the estimated pixel spacing and the slit width (full width at half maximum, FWHM) for the entire GOME wavelength range.

The method presented in this section has been successfully tested on several GOME solar spectra for many different windows. It is robust, and the nonlinear fitting generally converges within a few iteration steps, making the calibration process reasonably fast (a few seconds per window on a VAXstation 4000-60). The method has also been successfully applied to GOME earthshine radiance spectra at wavelengths between 370 and 410 nm where atmospheric absorptions are low.

Some additional work is required to optimize the window selection in order to get a better distribution across the different GOME channels and to avoid regions where the reference spectrum is corrupted by atmospheric features. The polynomial fit used to derive the final calibration curve over one channel currently uses only the shift information, but could be improved by also taking the retrieved pixel spacing information into consideration.

4. CALIBRATION BY CROSS CORRELATION

The cross-calibration procedure is derived from the method developed for fitting galaxy redshifts (Tonry & Davis, 1979). Briefly, segments of two spectra are cross correlated in Fourier transform space by transforming, multiplying the transforms, and back transforming the result. Studies on GOME data employ the XCSAO task of the RVSAO radial velocity package developed at the Smithsonian Astrophysical Observatory Telescope Data Center (http://tdc-www.harvard.edu/TDC.html) for IRAF (Kurtz et al., 1992). Because of the astrophysical origin of the software, the results (spectral shifts and their 1σ errors) are given in km s^{-1} and the GOME spectrum to be fitted is the "object." The reference spectrum is the "template." Wavelengths are input in Å. Options in XCSAO include cosine-bell apodization of the spectrum and the template (employed in these studies), and a choice of fitting functions to remove the continuum from the object and template. The GOME studies employ the "spline1" option, fitting polynomials of order 1-3, determined for each segment by experimentation. An example of the output from XCSAO is shown in Figure 4. In this case, a portion of the GOME radiance spectrum described below is cross correlated with the solar reference spectrum; a shift of -0.0086 ± 0.0011 nm is determined, *i.e.,* the GOME spectrum is at 0.0086 nm lower wavelength and must be shifted higher to correct it.

Spectral regions are selected and iterated by experimentation; a more extensive and systematic procedure would be necessary to parameterize an operational procedure. This study is limited to the determination of spectral shifts at particular portions of the spectra; an operational procedure would need to include polynomial fitting for the wavelength ranges of the various GOME channels. For each region, the GOME radiance and the irradiance are cross correlated with a solar reference spectrum that has been convolved with an appropriate slit function, as described below. The technique does not at present include a minimization process to optimize the slit function for minimum wavelength calibration error. Some optimization, described below, was done by hand iteration. For completeness, the GOME radiance and irradiance are also cross correlated, and a check made on the closure of the measured spectral shifts (the largest error in this closure is 0.0012 nm; it is usually substantially less than 0.001 nm).

The present study uses GOME data extracted from data product 60629054.lv1 (June 29, 1996), including the solar spectrum and radiance spectrum 1618 (SZA=81.92°, 52.99°S, 48.46°E). This spectrum was selected for very low albedo at 794 nm, as a difficult fitting choice and therefore a rigorous test of the method. Initial wavelength calibrations were made using the compound hyperbolic slit parameters from the concurrent version of GSLIT.LIB. Resulting calibration uncertainties are shown in Figure 5a. For reference, the uncertainty in the GOME solar reference spectrum and the limits for 0.02 GOME pixel have been included in this figure. Note particularly that the absolute wavelength accuracy at 361.5 nm, appropriate for fitting of OClO, is better than 0.001 nm and at 423 nm, appropriate for fitting of NO_2, it is 0.0013 nm.

A second set of calibrations were performed for the wavelength regions where uncertainties were relatively high. These used Gaussian slit functions for convolution of the solar reference spectrum, with widths determined from fitting in the earlier calibration by chi-square minimization. This led to a substantial improvement in the calibration at longer wavelengths, as shown in Figure 5b. An additional calibration point was added at this time, at 345 nm (the long-wavelength end of the O_3 Huggins bands).

Cross correlation of the two longest-wavelength segments was further refined by hand iteration of Gaussian slit widths. The improvement gained by this process is shown in Figure 5c. Another additional calibration point was added at this time, at 361.5 nm (appropriate for fitting of BrO in GOME spectra).

5. CONCLUSIONS

Absolute vacuum wavelength calibrations of GOME irradiance and radiance spectra are performed by two methods: (1) chi-square minimization of a merit function comparing GOME spectra to the GOME solar reference spectrum; (2) cross correlation with the GOME solar reference spectrum. Both methods are demonstrated to give calibration accurate to $\leq$0.002 nm (and $\leq$0.02 GOME pixel) except at the extreme ends of the GOME range and (for chi-square minimization) where the solar reference spectrum includes substantial residual atmospheric features. The calibration is particularly good at regions in the spectrum where concentrations of O_3, NO_2, BrO, and OClO are measured.

Neither method is yet an algorithm that might be considered for operational use. The following must be done before this can be the case:

- Multi-dimensional explorations must be made to optimize the choices of calibration wavelengths, segment widths, and parameters for the chi-square minimization or cross correlation task. This should substantially improve the overall calibration, particularly at the longest and shortest wavelengths.
- Appropriate polynomial coefficients to describe the calibration across the GOME channels must be derived.
- The procedures must be tested for robust, stable behavior over multiple orbits.

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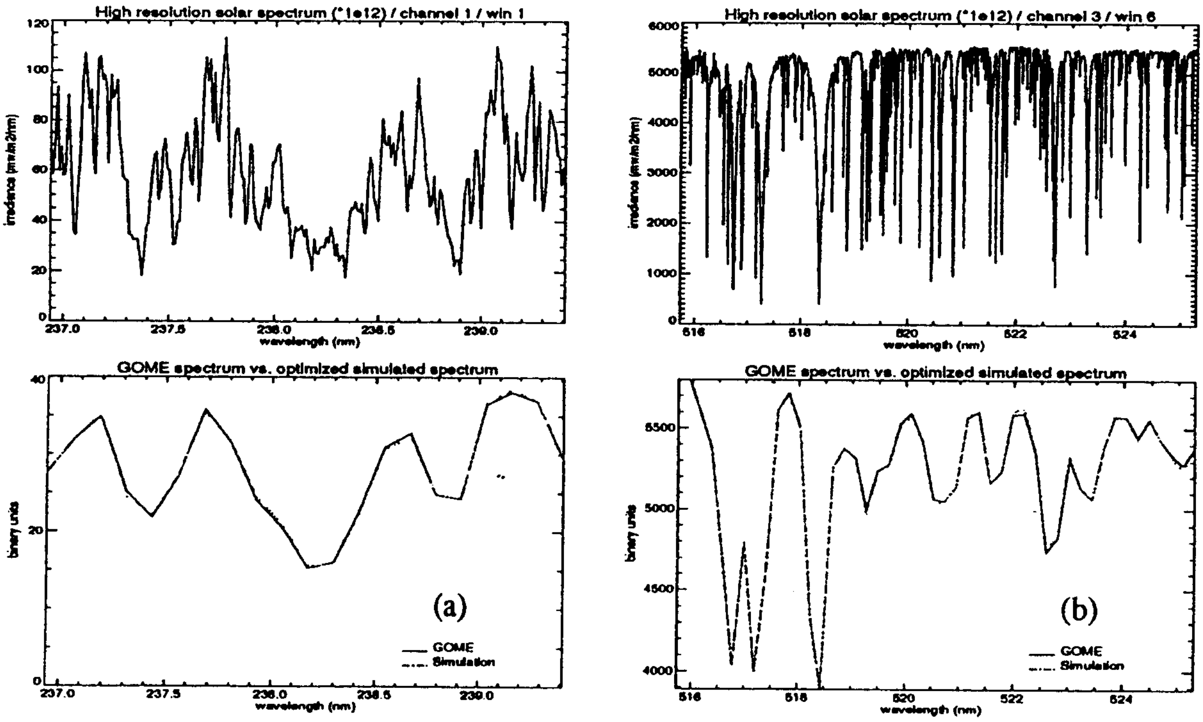

Figure 1: Fitting results for (a) channel 1, window 1 and (b) channel, 3 window 6. The upper plots show portions of the high resolution reference spectrum. The lower plots compare the GOME spectrum (solid line) with the simulated spectrum (dotted line) for optimized shift, squeeze and slit width parameters.

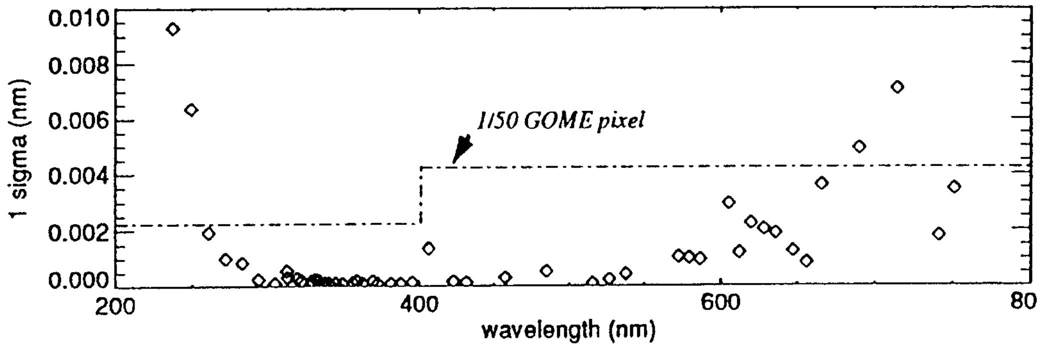

Figure 2: Absolute wavelength calibration uncertainties over the entire GOME wavelength range

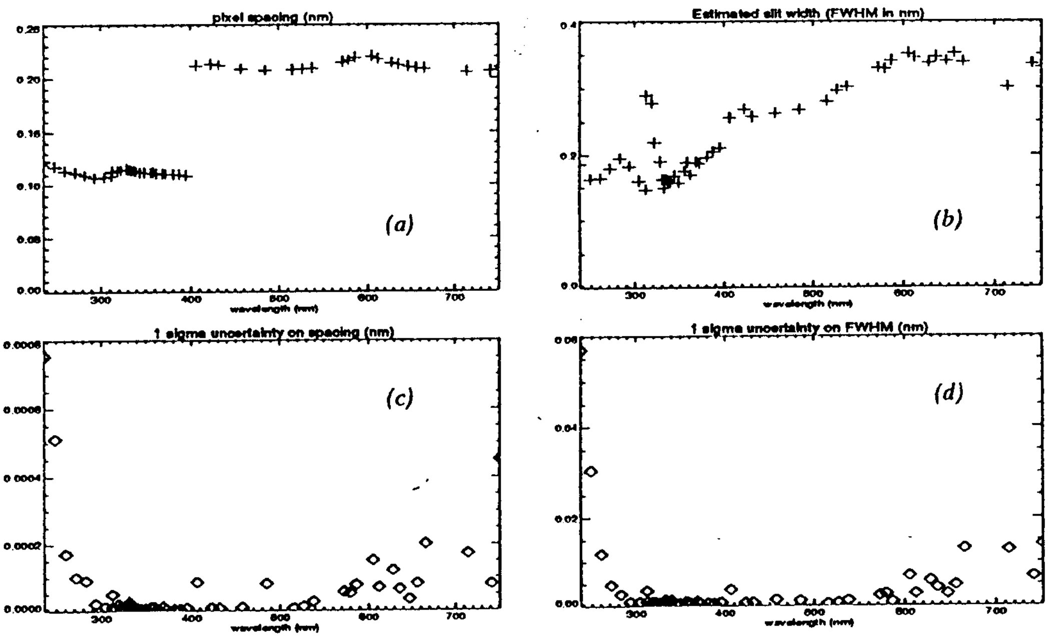

Figure 3: Estimated pixel spacing (a) and its 1 sigma uncertainty (b); estimated slit FWHM (c) and its 1 sigma uncertainty (d).

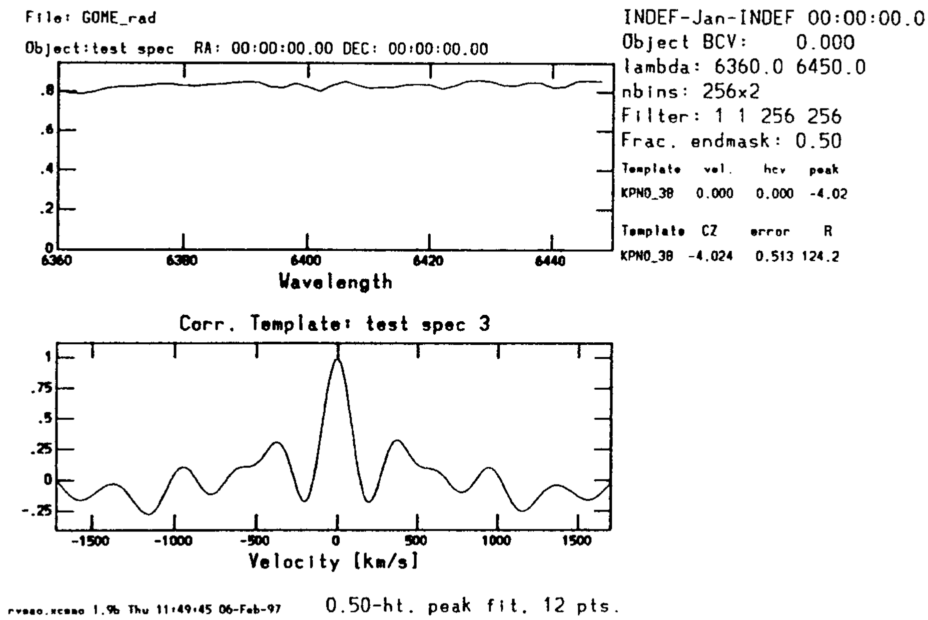

Figure 4: A segment of the GOME 60629054.1618 channel 4 spectrum correlated with the GOME solar reference spectrum. The redshift of -4.024±0.513 km s^{-1} corresponds to a GOME wavelength offset of -0.0086±0.0011 nm.

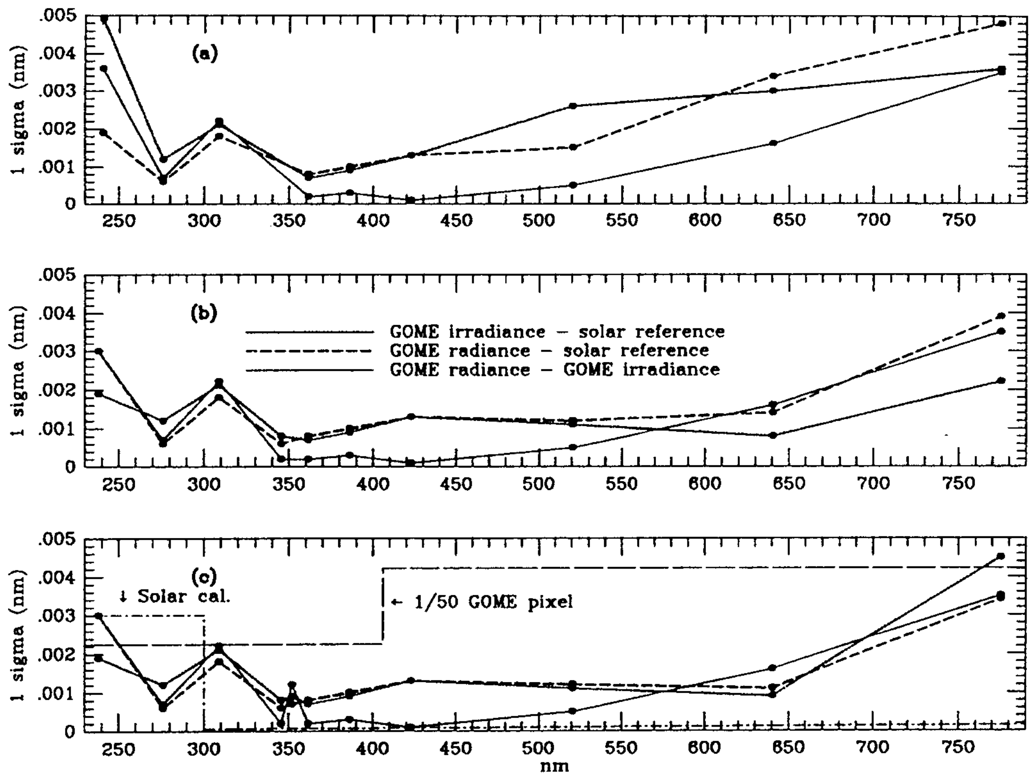

Figure 5: Absolute vacuum wavelength calibration uncertainties (1σ) for GOME. (a) Cross-correlation using the GOME solar reference spectrum convolved with the GOME compound hyperbolic slit function, with parameters from the current version of GSLIT.LIB. (b) Improvement of several points using Gaussian slit functions for convolution of the solar reference spectrum, with widths determined from fitting in the earlier calibration by chi-square minimization. (c) Further improvement of the two longest-wavelength points using hand iteration of Gaussian slit widths. The uncertainty in the GOME solar reference spectrum and the limits for 0.02 GOME pixel are included for reference.