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Comparing ground-level spectrally resolved solar UV measurements using various instruments: A technique resolving effects of wavelength shift and slit width

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Abstract. Spectrally resolved UV measurements are important for the study of biologically relevant UV in relation to changes in atmospheric parameters. The intercomparison of spectral instruments is essential as measurement techniques and calibrations are not standardized. The differences in slit functions cause large spectral variations when comparing the spectral readings directly. The method described, which compares spectral readings using different instruments, corrects for differences of wavelength calibrations and slit functions, and does not require knowledge of additional atmospheric parameters and UV-transfer model calculations. The wavelength alignment has an accuracy of 0.02 nm over the wavelength interval from 300-400 nm, and a reproducibility of 0.01 nm. The robustness of the methods and reproducibility of results are shown in the evaluation of a seven day intercomparison campaign with three different scanning spectroradiometers.

Introduction

A worldwide depletion of the ozone layer has been observed over the past decade (*Stolarski et al.*, 1992; *Herman et al.*, 1993). As a consequence, increased levels of UVB radiation at ground level are expected. UVB is the dominating wavelength range for adverse biological effects of solar UV exposure (*UNEP*, 1991). Risk assessments for the various effects require systematic spectrally resolved measurements of UV at ground level to obtain information on the changes in the spectral composition of the UV, and more particularly of the UVB. Because the spectral solar intensity varies by at least 3 to 4 orders of magnitude over no more than 20 nm around 300 nm, such measurements put high demands on the instrumental design and calibration. Thus to achieve precision in the order of a few per cent, wavelength calibration needs to be within 0.1 nm and very strong stray light rejection and precision irradiance calibrations are required.

A wide variety of instruments are used for measurements. It is also widely acknowledged that intercomparisons of spectral UV monitoring systems are required to assure the comparability of results (*Gardiner and Kirsch*, 1994). The fact that instruments vary in design and basic characteristics, like slit functions and stray light rejection, means that a direct intercomparison of spectral readings is not trivial. Evaluating instrumental intercomparisons in an EC project has shown that the analysis can best be based on ratios of time-synchronized spectral readings and that accounting for small errors in wavelength calibrations and differences in slit functions can improve comparability considerably (*Gardiner and Kirsch*, 1995). This paper will deal with a methodology for the intercomparison of measurement systems. Spectral shifts of the measured spectrum are evaluated on the basis of the solar spectrum's fine structure (Fraunhofer lines) (*Huber et al.*, 1993). An improved algorithm will be described and applied in this paper, along with an iterative deconvolution technique to improve comparability of measurements from systems with different slit functions.

The main advantage over previous methods is that knowledge of additional atmospheric parameters and UV-transfer model calculations are not required. The method was applied during a seven-day intercomparison campaign in August 1994 at the National Institute of Public Health and the Environment (RIVM) in Bilthoven. Measurements were obtained under varying cloud conditions.

Methods

Measurement Systems

The measurement systems are operated by the University of Innsbruck (UVI), the Royal Netherlands Meteorological Institute (KNMI) and the RIVM, and are described elsewhere (*Gardiner and Kirsch* 1994; 1995). All instruments consist of a double monochromator and a photomultiplier detection system. Table I summarizes the main characteristics of the instruments used in this study and the SUSIM extraterrestrial instrument (*Van Hoosier et al.*, 1988). The Full Width at Half Maximum (FWHM) of the slit functions are provided in table 1.

From August 2 to 11, 1994 spectral measurements were performed in Bilthoven (52.1 N, 5.2 E). Each group maintained its own calibration procedures. The instruments from UVI and RIVM were operated in fully synchronized scans for each half-hour from sunrise to sunset. Both were operated at the RIVM. The KNMI instrument was not fully synchronized; during the first days of the campaign it was operated at the KNMI (2 km from the RIVM site). The zenith angles of the analyzed data varied from 35-80°.

Shift Correction

Wavelength calibrations of the instruments are aligned by means of a new technique which compares the detailed structure of the measured ground-level spectrum with the extraterrestrial spectrum. To minimize influences due to atmospheric changes during a wavelength scan the comparison was applied considering the ratio:

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Table 1. Main characteristics of the measurement systems

instrument	monochromator	FWHM (nm)	wavelength step (nm)	wavelength range (nm)
UVI	Bentham	0.76	0.5	286-400
RIVM	Dilor	0.35	1.0	286-400
KNMI	MkIII Brewer	0.60	0.5	286-364
SUSIM	see Van Hoosier etal 1988	0.15	0.05	

$$R_M(\lambda) = \frac{2M(\lambda)}{M(\lambda - s) + M(\lambda + s)} \tag{1}$$

where: $R_M(\lambda)$ is the ratio of the measurement at wavelength λ, with two close neighbours; $M(\lambda)$, the measurement at wavelength λ, and s, the wavelength step between the central and two surrounding measurements (1 nm in this analysis).

The $R_M(\lambda)$ calculated above should be equal to a similar ratio obtained from extraterrestrial measurements with the same slitfunction [$R_E(\lambda)$]. Such extraterrestrial measurements are simulated using the SUSIM Extraterrestrial spectrum. Thereto, the SUSIM spectrum was deconvoluted applying the method described in the deconvolution section. Subsequently the deconvoluted result is convoluted with the slitfunction of the measurement. If the measured spectrum is slightly shifted, then $R_M(\lambda)$ equals $R_E(\lambda+\delta)$, where δ is the wavelength shift of the measured compared to the extraterrestrial spectrum. The wavelength shift is calculated by choosing a δ minimizing the sum of squared deviations of the ratios (σ^2):

$$\sigma = \sqrt{\frac{\sum_\lambda \left(\frac{R_M(\lambda)}{R_E(\lambda + \delta)} - 1\right)^2}{(n-1)}} \tag{2}$$

where: n-1 is the number of measured wavelengths included in the ratio calculations and where the sum is over a range of 16 nm, which unless stated otherwise starts at a wavelength of 332 nm.

Deconvolution; iterative method resolving effects of different slitfunctions

Measurements of spectral irradiance always include some stray light from nearby wavelengths. The slit function determines to what extent nearby wavelengths are recorded. The measured irradiance $M(\lambda)$ is a convolution of the slit function with the 'true' spectral irradiance $S(\lambda)$. The retrieval of the 'true' spectral irradiance from the measured spectrum can only be approximated by deconvolution techniques. We applied a simple iterative scheme. As a first estimate of the true spectrum, the zero-order deconvolution spectrum, we used the (deconvoluted) SUSIM extraterrestrial spectrum. This spectrum (S_0) is, of course, incorrect. A simulated measurement in iteration i [$M_i(\lambda)$] is calculated by a convolution of the simulation $S_i(\lambda)$ with the slitfunction:

$$M_i(\lambda) = \int f(\lambda' - \lambda)\, S_i(\lambda')\, d(\lambda') \tag{3}$$

where: $S_i(\lambda)$ is the deconvoluted spectrum at iteration i, and $f(\lambda-\lambda')$ represents the slit function of the instrument (we applied a triangular approximation, and normalized an integrated value of 1, using the FWHM bandwidth of the instruments).

We then calculated a correction spectrum $C_i(\lambda)$:

$$C_i(\lambda) = \frac{M_i(\lambda)}{M(\lambda)} \tag{4}$$

The correction spectrum is interpolated linearly between the measured wavelengths. The next iteration, $S_{i+1}(\lambda)$, of the deconvoluted spectrum is calculated by means of:

$$S_{i+1}(\lambda) = C_i(\lambda)\, S_i(\lambda) \tag{5}$$

The simulated measurements, usually within ten iterations, were very close to the original recorded spectrum and the iteration procedure was stopped. The last constructed spectrum was used as the deconvoluted spectrum. The deconvoluted spectrum was then convoluted with a standard triangular slit function with a FWHM of 1 nm to obtain a simulated measurement with a common slit function. Two readings from different instruments were compared by taking the ratios of the two simulated 1 nm FWHM spectra.

Results

Measurements were obtained with the three scanning instruments on seven consecutive days in Bilthoven from August 3-10, 1994. Figure 1 provides an example of two spectral readings at two different solar zenith angles on August 3 (36° and 69°). The spectral structure above 330 nm compares well with the extraterrestrial spectrum.

Figure 2 shows the deviation of ratios (σ) in the shift algorithm in relation to the shift in the spectrum for the three instruments. The three curves for the RIVM instrument illustrate the reproducibility of the obtained shift for readings at solar zenith angles of 36, 52 and 75°. An analysis of shifts in spectra from a single day showed that subsequent determinations for the RIVM instrument were reproduced with a SD of 0.005 nm; for the KNMI instru-

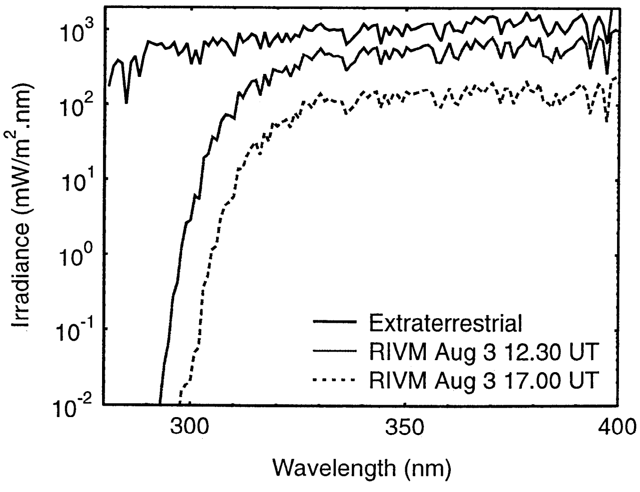

Figure 1. Extraterrestrial and ground-level solar spectra for sza of 36° and 69°.

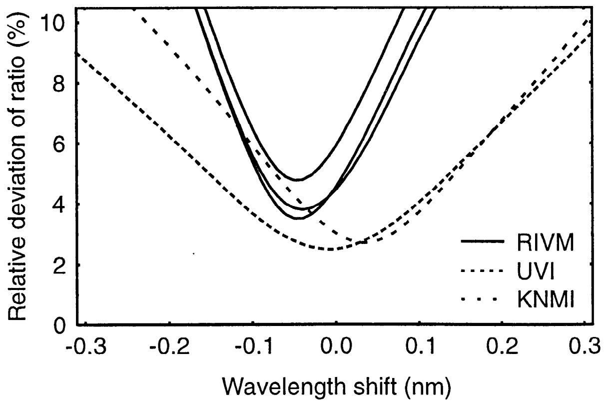

Figure 2. Determination of wavelength shift for 3 measured spectra with the RIVM instrument, and single measurements for UVI and KNMI instruments.

ment, 0.008 nm, and for the UVI instrument, 0.028 nm. Of the last-mentioned SD no more than maximally 0.015 nm could be attributed to the shift correction method. To investigate the wavelength dependence of wavelength alignment errors, the shift algorithm was applied with varying starting wavelengths. For the fixed 16 nm wavelength interval we varied the starting wavelengths from 300 to 380 nm. The algorithm was stable for the 330-380 nm range, with an SD of 0.0097 nm for the RIVM system and 0.014 nm for the UVI system. Larger deviations occur if the method is applied in the 300-330 nm region (0.05-0.07 nm maximally). A simulation showed that these deviations were fully attributable to the structure in ozone absorption. We concluded the wavelength shift over the full range from 300-380 nm to be stable, with an SD of maximally 0.02 nm. The stability of the shift algorithm in subsequent measurements is probably within 0.01 nm for these instruments.

Figure 3 shows a comparison between spectral readings from the RIVM and UVI instruments. The large structures of the uncorrected spectral ratios (dashed lines) of the spectra complicate a comparison. The structures are reproducible from scan to scan; this indicates that they are caused by the differences in slit functions of the instruments. We applied the shift correction and deconvolution method to the readings of both instruments and subsequently simulated readings of an instrument with a 1-nm slit function. Taking the ratios of the results reveals that this analysis reduces the structures more than fourfold (Figure 3, full line). Similar results were obtained when comparing the Brewer spectrophotometer from KNMI with the UVI instrument, although the structures in the uncorrected data deviate less due to the comparable slit widths of those instruments. Figure 4 shows the daily averaged ratios of the corrected spectra for the five days, where measurements covered the full day. The ratios are obtained dividing the measurement for each instrument by the average of the UVI and RIVM measurement. The large deviation with the KNMI Brewer spectrophotometer has been traced back to an erroneous factory irradiance calibration. The dotted curve indicates the result obtained for the KNMI/UVI ratio following a recalibration of the KNMI instrument (performed at KNMI in December 1994). The variation of ratios between days was no more than 1-1.5% for the fully synchronized measurements from UVI and RIVM, and no more than 1.7-2.3% for the comparison with readings from the KNMI instrument.

Discussion and Conclusions

Spectral monitoring of UV is performed worldwide with a variety of instruments. Calibration techniques and operational procedures vary. Therefore intercomparisons of instruments are essential in checking mutual calibration differences and achieving comparability of data obtained with different instruments at different locations. Previous papers and reports have dealt with various aspects of intercomparisons and subsequent data analysis (*McKenzie et al.*, 1993; *Koskela*, 1994; *Gardiner and Kirsch*, 1995). This study focuses on two aspects of the intercomparison of instruments: differences in wavelength calibrations and differences due to different slit functions. *Gardiner and Kirsch* (1995) have previously shown that corrections for these factors improve comparability of spectral readings considerably. Compared to their approach, the methods presented in this study have the advantage that no additional atmospheric data, or UV-transfer model calculations, are required for the evaluations.

The techniques provided in this study have been applied to seven days of data obtained in an intercomparison with three instruments. Over 120 spectral readings were

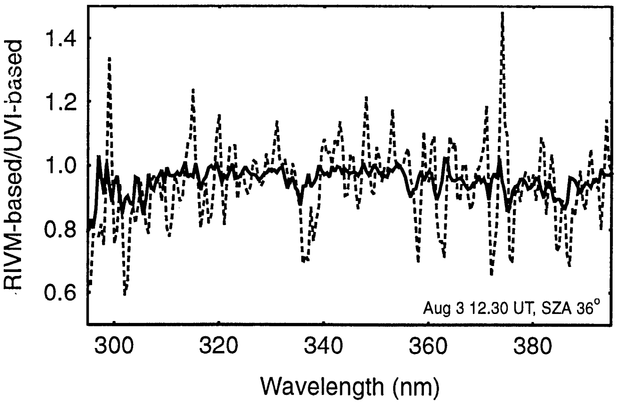

Figure 3. Ratio of RIVM and UVI measurements. Dashed: not corrected; Full: corrected for shift and slit functions.

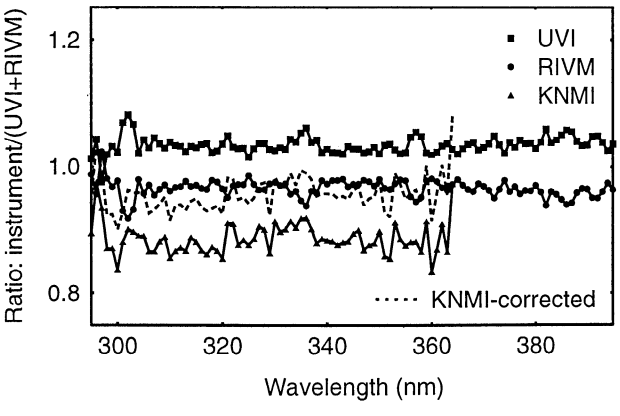

Figure 4. Shift and slit-function corrected ratios averaged over 5 full days. The result for each instrument is divided by the average spectrum from RIVM and UVI.

analyzed for each of the three instruments. Solar zenith angles varied from 35-80°. The results show that comparability of readings is particularly improved when deconvolution techniques are applied to correct for differences in slit functions. Under a variety of atmospheric conditions, from clear sky to almost fully overcast, we found very reproducible and stable results for the daily averaged corrected ratios of the spectral readings. The wavelength dependence of the spectral ratios was fairly flat in the 295-400 nm region (295-364 nm for the KNMI instrument). The overall absolute calibration differed, on average, by no more than 7% between UVI and RIVM, and nearly 10-15% between KNMI, and UVI and RIVM. Using a new calibration the deviation from RIVM was reduced to 1-3%, and the deviation from UVI to 7-10% (see Figure 4).

The remaining structures in the corrected spectral ratios are reproducible, indicating that further improvements of the methods might be possible by improved characterization of slit functions and/ or improved knowledge of the extraterrestrial spectrum. However, some structures might be due to atmospheric constituents.

The results prove the stability of the methods and instruments. The wavelength shift algorithm proved to be very stable under varying atmospheric conditions. The Standard Deviation of shift determinations for subsequent spectra during a day was around 0.01 nm. Wavelength dependent alignment errors can also be detected when the wavelength shift algorithm is applied with different wavelength intervals. In order to give useful results this approach requires the assumption that the SUSIM extraterrestrial spectrum does not have significant wavelength dependent errors of the alignment. This assumption is fully supported by the wavelength independent shift results obtained with the UVI and RIVM instruments. Over the range from 330-380 nm the Standard Deviations were 0.0097 nm for the RIVM instrument and 0.014 nm for the UVI instrument. Application of the shift algorithm in the spectral range from 300-330 nm shows larger deviations (maximally 0.05-0.07 nm), which are caused by the finestructures in the ozone absorption spectrum. Thus, application of the shift algorithm in the range below 330 nm requires modelled ozone absorption.

Two relevant advantages of the methods presented in this study are that they can be easily applied during a campaign shortly after the spectral measurements, and that results are fully independent of UV-transfer model calculations. The techniques applied here can serve as a valuable tool in routine monitoring, future intercomparisons and contribute to the comparability of spectral datasets.

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