

Spike detection and correction in Brewer spectroradiometer ultraviolet spectra

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Abstract. The occurrence of spikes in Brewer UV spectra is studied. Use is made of continuous measurement data over several years, comprising more than 90,000 spectra, from one single-monochromator and two double-monochromator Brewers. It is shown that the double monochromators, especially, may suffer from more than 200 spikes per ~5000 annual spectra. The spikes are not always randomly distributed over the wavelength range. The single monochromator is found to have an annual average of only 36 spikes above 300 nm, but it is noted that there were a significant number of spikes at shorter wavelengths, indicating possible bias in the stray light correction unless taken into consideration. The error caused by noncorrected spikes varies greatly from case to case. In an intensive study of 150 spectra measured during one summer week, the effect of one moderate-size spike was found to be more than 5% on a DNA action dose rate and close to 1% on a DNA action daily dose. When high accuracy of *in situ* UV measurements is required, our results suggest a need to remove spikes from the spectra. A simple statistical approach is employed. The method is applicable to any single- or double-monochromator Brewer spectroradiometer. However, under rapidly changing cloudiness it can be difficult to distinguish between noise spikes and the variation in irradiance due to changes in the state of the sky. Our data show that ancillary radiation measurements may be necessary to interpret the data correctly. © 2003 Society of Photo-Optical Instrumentation Engineers. [DOI: 10.1117/1.1569492]

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1 Introduction

Several error sources and uncertainties are involved in the measurement of UV radiation.¹ Recently much effort has been put into identifying and correcting errors due to, e.g., an imperfect cosine response²⁻⁵ and temperature dependency.^{6,7} One of the most common instruments used to measure spectral UV irradiance is the Brewer spectroradiometer.⁸ These are operated worldwide, and therefore have the potential to act as references for satellite data validation (see, e.g., Ref. 9). In this paper, data from two types of Brewer instruments are included, one single monochromator (Brewer MKII), and two double monochromators (MKIII). In addition to the version differences, properties may vary from one specific instrument to another. The occurrence and effect of spikes in the UV spectra were studied. By a spike we mean an anomalous number of counts recorded in one wavelength channel causing an abrupt upward or downward change in value that does not originate from the true radiation signal [Fig. 1(a)]. We have recorded downward spikes, for example, in lamp scans measured in the darkroom, and spikes occur in sky measurements as well.

The origin of the spikes is not fully understood. Diverse causes have been suggested, from hardware or software to the effect of cosmic radiation. Allaart¹⁰ studied the occurrence of spikes in Brewer MKIII #100, and found them not

to occur randomly; on the basis of their data he concluded that spikes are most probably caused by a software error. On the other hand, according to Gröbner, with their new double Brewer in operation since June 2001, using the new electronics, there have been no spikes in the data so far.¹¹

Here, a simple but effective statistical method is formulated and used to identify and correct spikes in Brewer UV spectra. Our main goal was to remove spikes and correct data, minimizing the potential error. The methodology presented here is applicable for any single- or double-monochromator Brewer spectroradiometer. Other approaches to spike removal exist, but all the methods are slightly different, as noted in Sec. 3.2. Bernhard et al.¹² demonstrated the usefulness of the ratio spectra method for the detection of several instrumental malfunctions, including spikes or distortions in an instrument's signal. In their method, a set of spectra measured throughout the day are ratioed against a reference spectrum from the same instrument. In addition to these methods, the algorithm used by the World Meteorological Organization (WMO) World Ozone and Ultraviolet Radiation Data Center¹³ (WOUDC) in Toronto, Canada, to process data from level 0 (raw data) to level 1, applies spike detection and correction. Data that are noisy from wavelength to wavelength are corrected and flagged.

Variable cloudiness can present problems for spike removal. When measuring UV spectra, we receive spectral

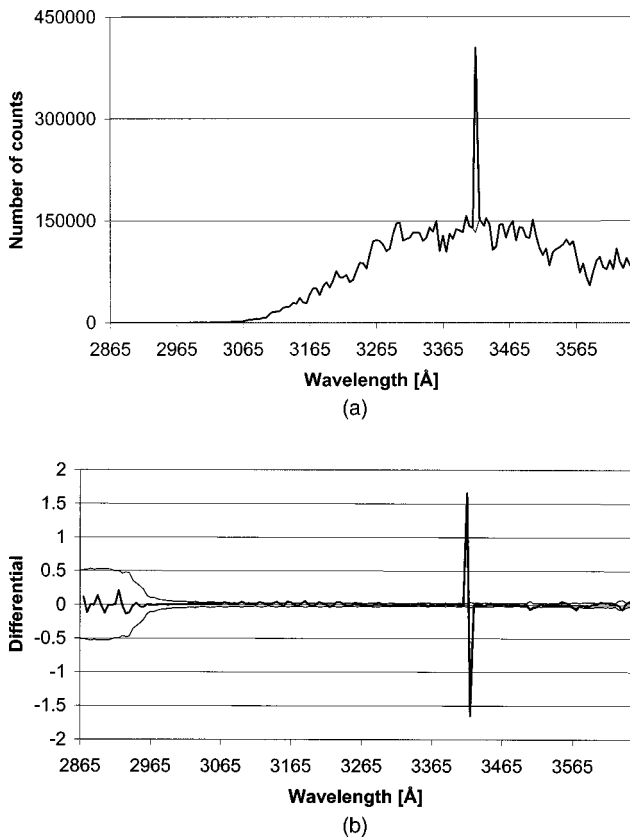


Fig. 1 (a) Example of a spike in a Brewer 107 spectrum measured on May 8, 1999 (thick line), and the corrected value (thin line), with the number of counts as a function of wavelength in angstroms, and (b) the same data calculated as ΔR (thick line) together with ± 2.6 sigma curves (thin lines) calculated for each wavelength based on a 2-yr data set (see text for details).

information in variable unpredictable cloud conditions that can cause 60 to 70% changes in global irradiance within seconds.¹⁴ This problem is especially significant in instruments that have a relatively long measurement time for each wavelength channel, such as Brewer spectroradiometers. For this instrument, one scan takes several minutes, and measurement in one channel typically takes 2.5 s. This relative slowness can induce additional problems in how to distinguish spikes from the variation in irradiance due to changes in the state of the sky. Our data showed that ancillary radiation measurements may be necessary to interpret the data correctly.

2 Materials and Methods

2.1 Spectroradiometer Measurements

The Finnish Meteorological Institute (FMI) makes continuous measurements of spectral UV irradiance in southern and northern Finland using two Brewer instruments, a double monochromator MKIII #107 at Jokioinen (60°44'N, 23°30'E) since April 1995, and a single monochromator MKII #037 at Sodankylä (67°22'N, 26°39'E) with calibrated data since June 1990. The Swedish Meteorological and Hydrological Institute (SMHI) has measured UV irradiance continuously at Norrköping (58°35'N, 16°09'E) with Brewer MKIII #128 since 1996.

The spectral range of the MKIII instrument is 286.5 to 365.0 nm in 0.5-nm steps, while for the MKII it is 290.0 to 325.0 nm in 0.5-nm steps. A detailed description of the instruments can be found from the manufacturer (Kipp and Zonen).

In this analysis, more than 90,000 spectra were studied. This included all the available measured data of about 5000 spectra annually for Brewer MKIII #107 for the period 1996 to 2001, and for MKII #037 for the period 1991 to 2001, as well as the annual data from 1999 and 2000 for MKIII #128, to investigate possible differences between the double-monochromator instruments. The aim was to study the frequency of occurrence and wavelength distribution of spikes in the spectra, whether there is any difference between the spikes occurring in single or double monochromators, and whether the removal of the spikes has any effect on the products calculated from the data. A one-week period (May 3 to May 9, 1999) of about 150 MKIII #107 spectra was studied in more detail to investigate whether spike removal could have any significant effect on dose rates (nonweighted and weighted spectral integrals) or daily doses (dose rates integrated over one day).

Furthermore, to study whether a sudden extensive change in the measured irradiance is due rather to real changes in the irradiance than to an instrumental artifact, synchronized broadband and spectral UV measurements were used. These were obtained at Jokioinen by using the Brewer #107 and a Solar Light Model 501A erythemal UV detector connected to a Vaisala QLI-50 data logger. The spectroradiometer system fulfills WMO recommendations for category S-2 spectral measurements.¹⁵ The time constant of the broadband detector is 0.5 s for a 95% response, which is sufficient for the detection of rapid changes of cloudiness. A more detailed description of the instrument can be obtained from the manufacturer (Solar Light).

2.2 Removing Spikes

In many measurements, the problem of identifying and correcting spikes is common, but it is not trivial in radiation measurements. This is due to the considerable variation of solar irradiance with wavelength and the variation in the terrestrial solar spectrum with time under conditions of rapidly changing cloudiness. Hence, it is difficult to distinguish between noise spikes and the variation in irradiance due to changes in the state of the sky. It is also important to use spike removal from the very beginning of the spectrum to prevent the stray light correction becoming distorted by spikes. In particular, it can be assumed that no radiation below 292 nm will penetrate the atmosphere at the locations considered in this paper. The recorded values at the very beginning of the spectrum are used only as a measure of the unwanted stray light in the instrument's monochromator, to be removed from all wavelength channels.

The method used here is based on the differences in relative changes in the spectra, not in absolute values. The term "data" refers here to raw spectral data in counts, i.e., data not corrected for dark current, dead time, or instrument response, and often presented as a function of wavelength in angstroms rather than nanometers.

A simple statistical method was used to identify the spikes in Brewer UV spectra. To start with, a clear-sky reference spectrum is required. Since only relative changes

are calculated, the reference can be a single clear-sky raw spectrum or an average spectrum of several midday clear-sky spike-corrected raw spectra. We calculated the reference from all available clear-sky spectra with a solar zenith angle (SZA) smaller than 60 deg, using 2 yr of measured data. The total number of such spectra was 75. Second, the standard deviation of ΔR_i [see Eq. (2)] at each wavelength, based on a large data set, is computed. We used 2 yr of data (1999 and 2000) with 11,212 spectra to get an estimate of the variability of ΔR_i . Third, spectral ratios of raw counts divided by the reference counts are computed

$$R_i = \frac{C_i}{C_i^{\text{ref}}}, \quad (1)$$

where i denotes a single 0.5-nm-wide channel. Fourth, the differences in these ratios between neighboring channels, e.g., for i and $i-1$, are calculated, as follows:

$$\Delta R_i = R_i - R_{i-1} = \frac{C_i}{C_i^{\text{ref}}} - \frac{C_{i-1}}{C_{i-1}^{\text{ref}}}. \quad (2)$$

Last, the ratio differences ΔR_i and ΔR_{i+1} are compared against the chosen confidence level. According to our definition of spikes, a spike exists if ΔR_i exceeds the confidence level in a given channel in one direction and the next channel in the opposite direction, as given by

$$\Delta R_i > a\sigma(\Delta R_i) \quad \text{and} \quad \Delta R_{i+1} < -a\sigma(\Delta R_i) \quad (3a)$$

or

$$\Delta R_i < -a\sigma(\Delta R_i) \quad \text{and} \quad \Delta R_{i+1} > a\sigma(\Delta R_i), \quad (3b)$$

where, e.g., the constant $a=3$ corresponds to an estimate of the 99.74% probability using the temporal standard deviation $\sigma(\Delta R_i)$ calculated for each wavelength.

In practice, the choice of the constant a regulates what kinds of spikes are likely to be found. For example, when $a=5$, some small spikes may be unidentified, while they would be found with $a=2.6$. With a measurement time of several seconds per channel, it may be difficult to distinguish between clearly artificial spikes and cloud-induced shape distortions. To avoid correcting a real variability caused, e.g., by rapidly changing clouds, an additional rule can be used. This can be important if a small constant a value is used. The rule may be, for example, that a spike is removed only if the ratio of counts divided by the corrected counts exceeds 1.5 or is less than 0.5 (the 50% rule). The *ad hoc* setting of these parameters depends on the data. The ratio of detected versus corrected counts can give useful additional information. For example, for #107 data from 1996 to 2001 with 2.6 sigma and a 10% rule, we found that the spectral distortions were grouped into a distribution having two maxima: one around the ratio (detected/corrected)=1, and the other around 3 (Fig. 2). There was a gap in the number of cases between these maxima, which indicates that spectral distortions around these two maxima may have different origins. The smaller spectral distortions at the first maximum may originate from, e.g., fast changes in the cloud optical depth, cloud

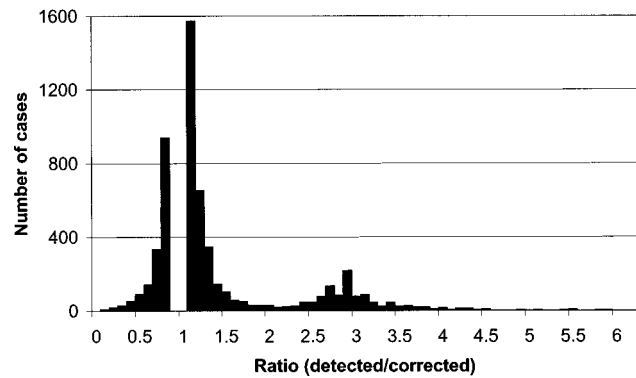


Fig. 2 Size distribution of the ratio detected-to-corrected counts with the 2.6 sigma and 10% rule for #107 data of the period of 1996 to 2001 (see text for details). The first maximum around the value one is due to both the real variability in the measured signal and the small distortions below 3000 Å. The second maximum near the value three originates from noise spikes with a typical ratio size of 2.5 to 3.5.

reflections of the direct beam, an SNR problem, or cases below 3000 Å. The second maximum consists of larger distortions that must be considered as noise spikes and must be corrected. The correction of small distortions is questionable; one approach might be to flag them in the data analysis. We also found that whether we used for those data the 50% rule or the 100% rule, the number of spikes as a function of wavelength remained almost the same. This supports the fact that for #107 the 50% rule was powerful enough to detect the noise spikes but that the result was not contaminated by changes in cloudiness.

The first and last wavelengths are not included in this analysis, since they do not have two neighboring channels. This will cause only a minor error for the first channel, because of its use solely for the stray light correction. The error in the last channel can be completely avoided either by excluding the last channel from the analysis, or by setting a quality control value for it, if desired. One possibility is to use nonpairwise comparison. The spikes are so rare that two consecutive spikes are assumed not to exist.

The new corrected value for the removed spike is calculated using values in neighboring channels, and the reference spectrum value, as given by

$$C_i^{\text{corrected}} = 0.5 \left(\frac{C_{i-1}}{C_{i-1}^{\text{ref}}} + \frac{C_{i+1}}{C_{i+1}^{\text{ref}}} \right) C_i^{\text{ref}}. \quad (4)$$

In this way, we preserve the characteristic shape and fine structure of the spectrum better than by using the average of the neighboring channel values as such.

3 Results and Discussion

3.1 Spikes in Single and Double Monochromators

We compared possible differences in the occurrence of spikes between single and double monochromators. From the experience gained in operating these instruments, it was suspected that the single monochromator would have a low frequency of spikes. Earlier it was reported that, due to stray light problems, the single-monochromator Brewer is not capable of recording accurate solar spectra at

Table 1 Spikes in the single-monochromator Brewer MKII #037 data at 290 to 299.5 nm and at 300 to 325 nm with the 2.6 sigma and 50% rule (see text for details).

Year	Number of spectra	Number of spikes at 290 to 299.5 nm	Number of spikes at 300 to 325 nm	Spikes per wavelength at 300 to 325 nm
1991	5156	43	29	0–3
1992	4729	44	9	0–2
1993	4922	60	44	0–3 except 9 at 316 nm
1994	5027	17	71	0–4 except 11 at 302 nm
1995	5308	25	99	0–5 except 6 at 302 nm
1996	5022	65	23	0–2
1997	5606	59	49	0–5
1998	4823	25	30	0–4 except 6 at 316 nm
1999	5897	30	13	0–2
2000	5850	22	7	0–1
2001	5665	20	23	0–5

wavelengths¹⁶ less than about 300 nm. For the single MKII #037 data at 300 to 325 nm, the number of spikes detected in 1999 and 2000 with the 2.6 sigma and 50% rule was only from zero to two spikes per wavelength, with totals of 13 and 7 spikes per year, respectively (Table 1). In 2001, there were 23 spikes with zero to five spikes per wavelength. The power supply was changed on January 10, 2001. For earlier data, the number of spikes has varied between 9 and 99 spikes annually with approximately 1% of the measured spectra suffering from a spike. However, the number of spikes below 300 nm was notable (Table 1). Although the level of the measured signal at shorter wavelengths is small, our results suggest a possible error source for the stray light correction unless the spikes are removed.

On the basis of earlier experience in operating the instruments, the double-monochromator data were expected to include more spikes than those for the single monochromator. For the 6-yr data set of Brewer MKIII #107 spectra between 300 and 365 nm with the 2.6 sigma and 50% rule, the number of spikes varied from 125 to 246 annually. Hence, an average of 4% of the measured spectra suffered from a noise spike. For #128, the corresponding results were 265 spikes in 1999 and 255 in 2000, which corresponds to ~7% of the spectra [Fig. 3(a)]. Larger spikes, detected with 5 sigma, were 165 in 1999 and 171 in 2000, i.e., in 4% of the #128 spectra [Fig. 3(b)]. These results confirm the assumption that the single-monochromator data did not suffer from spikes to the same extent as those of the double monochromator.

3.2 Other Spike Removal Methods

As mentioned earlier, other methods exist to detect and correct spikes. These unpublished approaches are all slightly different. The simple threshold method¹⁷ compares

$$\frac{C_i^{\text{ref}}}{C_{i-1}^{\text{ref}}} - \frac{C_i}{C_{i-1}} > \text{threshold value}, \quad (5)$$

where the limit is 1, if $C_i < 200$ (number of the measured counts), and 0.5 if $C_i > 200$. Then the new value will be

$$C_i = C_i^{\text{ref}} C_{i-1}. \quad (6)$$

In another approach,¹⁸ the comparison is

$$\frac{C_i}{C_{i-1}} > \frac{C_i^{\text{ref}}}{C_{i-1}^{\text{ref}}} + 3\sigma \left(\frac{C_i^{\text{ref}}}{C_{i-1}^{\text{ref}}} \right) \quad \text{or} \quad \frac{C_i}{C_{i-1}} < \frac{C_i^{\text{ref}}}{C_{i-1}^{\text{ref}}} - 3\sigma \left(\frac{C_i^{\text{ref}}}{C_{i-1}^{\text{ref}}} \right), \quad (7)$$

and the corrected value will be

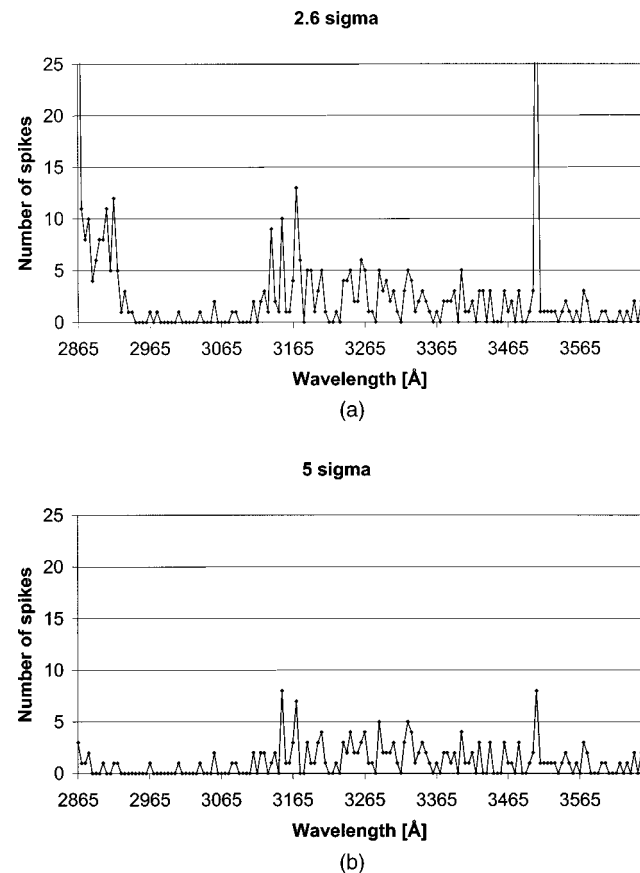


Fig. 3 Number of spikes in the double-monochromator Brewer #128 data in 2000 as a function of wavelength in angstroms detected with (a) the 2.6 sigma and 50% rule and (b) the 5 sigma and 50% rule (see text for details).

$$C_i = C_i^{\text{ref}} C_{i-1}. \quad (8)$$

In the third method,¹⁹ the standard deviation is calculated over the wavelength range of the spectrum that is studied:

$$\frac{C_{i+1}}{C_{i+1}^{\text{ref}}} - \frac{C_i}{C_i^{\text{ref}}} > 5\sigma(\Delta R_i) \quad \text{or} \quad \frac{C_{i+1}}{C_{i+1}^{\text{ref}}} - \frac{C_i}{C_i^{\text{ref}}} < -5\sigma(\Delta R_i), \quad (9)$$

and the neighboring channels must have a pairwise overshoot of opposite sign. The spike is corrected by first fitting a 2-deg polynomial to the ratios and then multiplying the resulting value by the value of the reference spectrum.

As far as the detection of spikes is concerned, our approach is closest to that of Eq. (9). In both cases, to detect a spike, it is necessary that the signal first increases in one channel and then decreases in the next channel (or vice versa). This assumption works well with the actual measurement data under variable cloudiness. Also, in both cases, the calculated differences of $C_{j+1}/C_{i+1}^{\text{ref}} - C_i/C_i^{\text{ref}}$ approach zero [Fig. 1(b)], in which case the spikes are easily detected. The difference between our method and the approach of Eq. (9) is that we use a large data set (2 yr of measured spectra) to calculate once the temporal standard deviation of ΔR_i [see Eq. (2)], which is used to identify spikes. Our method works at all wavelengths. In the other method, the standard deviation is calculated in wavelength space from the data under study, and the first six channels are often excluded from the analysis. In addition, in calculating the new value, we do not fit a polynomial, but simply replace the value on the basis of the neighboring channels and reference spectrum values to reproduce the Fraunhofer structure in the corrected spectra. Nevertheless, a detailed comparison of different methods for spike detection is beyond the scope of this paper.

3.3 Distribution of Spikes Over the Measurement Range

It was our hypothesis that the spikes would be quite randomly distributed over the measured wavelength range. For MKIII #107, this was the case for the first three measurement years from 1996 to 1998 [data for 1998 shown in Fig. 4(a)]. In the following years, the spikes were concentrated at certain wavelengths. In 1999 this included three areas, in the range 340 to 344 nm, at 348, and at 350 nm [Fig. 4(b)]. Of these, the spikes at 350 nm at least may be connected with the changing of the slit there during the measurement scan. Spectra measured in 2000 and 2001 (data not presented here) had a common spike problem at around 350 to 355 nm, but it was different than that in the year 1999. For MKIII #128, during both the years 1999 and 2000 there were in general from zero to six spikes per wavelength, but more spikes were concentrated at 315, 317, and 350.5 nm as detected both with the 2.6 sigma or 5 sigma thresholds (data for 2000 presented in Fig. 3). For the MKII #037 data, the spikes were more clearly randomly distributed, with only two wavelengths—302 nm and 316 nm—showing some spike concentrations in the 11-yr data set (Table 1).

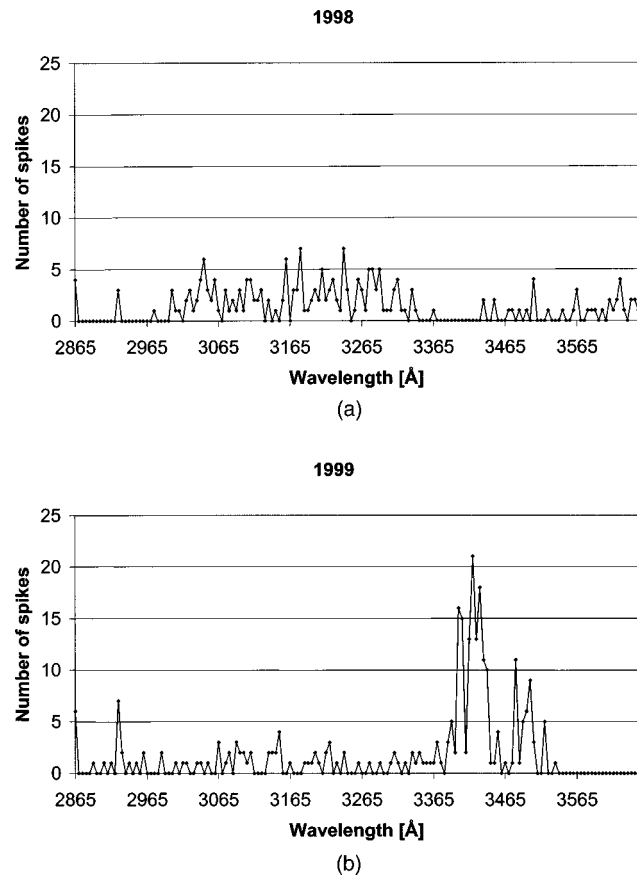


Fig. 4 Number of spikes in the double-monochromator Brewer #107 data (a) in 1998 and (b) in 1999, as a function of wavelength in angstroms detected with the 2.6 sigma and 50% rule (see text for details).

The position of the concentrated spikes might be an indication of the general functionality of the instruments, either of the software or hardware.

3.4 Effect of Spikes on Calculated Dose Rates and Daily Doses

A 1-week period (May 3 to 9, 1999) of Brewer MKIII #107 data with about 150 spectra was randomly selected to represent a typical week in spring or summer. The data were thoroughly studied case by case to determine whether spike removal would have a notable effect on nonweighted and weighted dose rates or daily doses. In that data set, using the 2.6 sigma and 50% rule, there were zero to two spikes per day with a total number of seven spikes. One moderate spike (the ratio of uncorrected counts to corrected counts was 2.7), detected on the May 9 at 318.5 nm, had the following effects on dose rates: 5.5% on DNA action, 2.9% on Commission Internationale de l'Éclairage (CIE) erythema, and 0.5% on nonweighted UV-A (Table 2). The effects on the daily doses were 0.8% on DNA action, 0.4% on CIE erythema, and 0.1% on nonweighted UV-A. Our results demonstrate that the error in weighted integrals caused by moderate spikes can be as much as several percent, although the uncertainty due to noise is often reduced when biologically weighted irradiances are calculated,¹ diminishing the effect of small spikes. The effect of the spikes de-

Table 2 The differences in percent between uncorrected and spike-corrected (with the 2.6 sigma and 50% rule) Brewer MKIII #107 spectra for nonweighted UV-A and UV-B, as well as for DNA and CIE erythral weighted dose rates, intensive study period May 3 to 9, 1999.

Day in 1999	Time (UTC)	Spike detected at (nm)	Nonweighted UV-A	Nonweighted UV-B	DNA action	CIE erythral action
May 3	—	—	—	—	—	—
May 4	10:38	350	0.1	0.0	0.3	0.2
May 5	—	—	—	—	—	—
May 6	6:52	340	2.0	0.0	0.2	1.2
May 7	5:15	350	1.2	0.0	0.1	0.7
	17:55	340	1.2	0.0	0.3	1.6
May 8	6:28	341.5	1.9	0.0	0.1	1.2
May 9	2:01	337	0.0	0.0	0.0	0.0
	8:26	318.5	0.5	0.0	5.5	2.9

depends on their size and location in the measured spectrum, and the corresponding action spectrum: a spike occurring at a wavelength with higher weight will result in a larger error. The effect therefore varies greatly from case to case.

3.5 Spikes versus Rapid Changes in the Irradiance Due to Clouds

The functionality of the spike detection and correction method was studied by comparing our method with the threshold method [Eq. (5)] for the years 1999 to 2000. Ancillary broadband UV data was used as an independent indicator of the true changes in the solar irradiance. In general, the visually detectable spikes were also detected by both of the programs, with some minor differences. One obvious difference between the methods was that, due to its different spike definition, the threshold method suggested spikes, when a change in irradiance, probably caused by fast changes in cloud transmission, was actually in question. The threshold method is based on the use of interactive software, and it is the user who decides, on the basis of the plotted figures, whether to accept the correction suggested by the program.

To conclude, there are natural situations in which a rapid change of cloudiness can distort the shape of the spectrum in a way similar to that of a spike. An example of this is given in Fig. 5. Here both the visual inspection of the spectral irradiance and the software suggest the presence of a spike that needs to be corrected. Only the parallel analysis of the ancillary data indicates that no correction is needed, because there is a corresponding sudden change in irradiance in the broadband radiometer output. This case clearly points out the usefulness of synchronized ancillary measurements for UV data processing, as stated in Seckmeyer et al.¹⁵

4 Summary and Conclusions

Our aim was to study the frequency and spectral distribution of spikes in Brewer single- and double-monochromator data. We also wanted to quantify the influence of these spikes on the calculated dose rates and doses. It was found that the effect on doses and dose rates varies from case to case and that its magnitude can be as much as several percent. When highly accurate *in situ* UV measurements are

required, our results suggest an obvious need to detect and correct spikes from the data. The fact that spikes were not randomly distributed over the wavelength range suggested that the origin of the spikes is not random electrical noise. Spikes were more frequent in the double-monochromator data than in that of the single monochromator. This gives

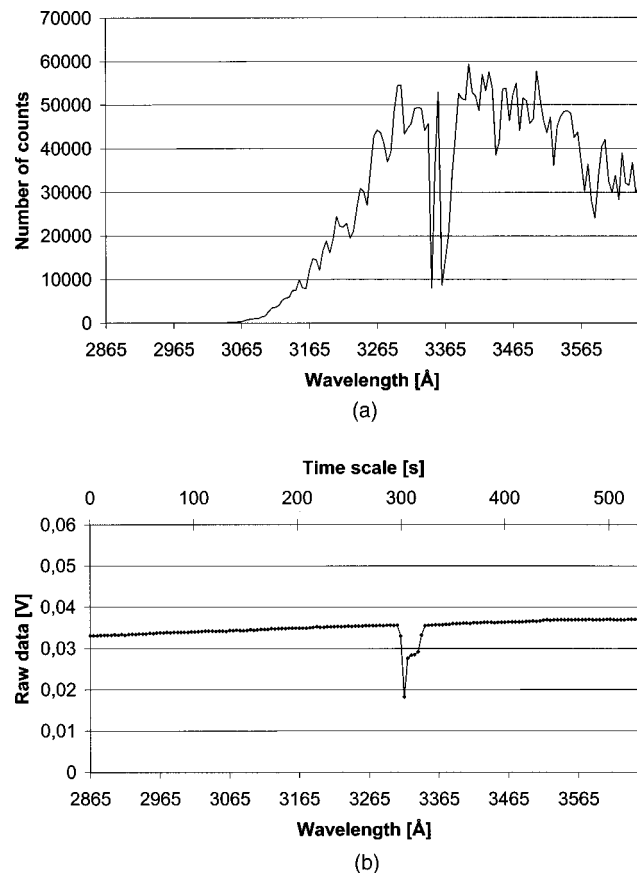


Fig. 5 (a) Brewer #107 UV spectrum with a strong decrease in raw counts at 3345 and 3360 Å, August 8, 1999. (b) Time-synchronized raw data in volts recorded by a SL-501 broadband UV radiometer. The x axis shows both the time of the broadband meter measurement and in particular the corresponding wavelength position in angstroms of the spectroradiometer.

some indication that the spike problem could, at least to some extent, be related to properties that are different between the instrument versions. The statistics presented are not directly applicable to other instruments of the same type because properties may vary from one specific instrument to another. However, the method presented in this paper is applicable to other instruments as well, and is recommended to save the bookkeeping of the spike correction procedure. It can be used as a quality control tool for Brewer measurements.

Under conditions of rapidly changing cloudiness, it may be difficult to distinguish between noise spikes and the variation in irradiance due to changes in the state of the sky. This problem is particularly significant for instruments that have a relatively long measurement time for one wavelength channel, such as Brewer spectroradiometers. Our data showed that ancillary radiation measurements may be necessary to interpret the data correctly.

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