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Accuracy of total ozone retrieval from NOAA SBUV/2 measurements: Impact of instrument performance

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Abstract. The National Oceanic and Atmospheric Administration/National Environmental Satellite Data and Information Service (NOAA/NESDIS) has been collecting and evaluating the solar backscattered ultraviolet (SBUV/2) instrument data from NOAA 9 and NOAA 11 spacecraft since March 1985. Over 5 years (March 1985 to October 1990) of NOAA 9 (version 5.0) and over 4 years (January 1989 to June 1993) of NOAA 11 (version 6.0) reprocessed data are now available to the scientific community to study geophysical phenomena involving ozone. This paper examines the impact of the instrument performance on total ozone retrieval from the two instruments. We estimate that at the end of October 1990 the total postlaunch error for NOAA 9 due to instrument alone is −2.2%. A significant fraction of this error (−1.9%) is due to diffuser degradation which is not accounted for in the version 5 reprocessing. The estimate for NOAA 11 total postlaunch instrument error, at the end of June 1993, is −0.4%.

1. Introduction

The first solar backscattered ultraviolet (SBUV/2) instrument was launched December 12, 1984, aboard the NOAA 9 spacecraft to measure global ozone for the purpose of detecting and monitoring stratospheric ozone changes. A second SBUV/2 instrument was launched September 24, 1988, aboard the NOAA 11 spacecraft to replace the SBUV/2 instrument on the aging NOAA 9 spacecraft and to provide continuity in the ozone measurements. Both SBUV/2 instruments are similar to their predecessor SBUV instrument that was flown on the Nimbus 7 spacecraft [*Heath et al.*, 1975] and to a lesser extent the BUV instrument that was flown on the Nimbus 4 spacecraft.

As a part of its mission, National Oceanic and Atmospheric Administration (NOAA) has been collecting, processing, and analyzing the SBUV/2 data from the NOAA 9 and NOAA 11 spacecraft. Over 5 years (March 1985 to October 1990) of NOAA 9 (version 5.0) and over 4 years (January 1989 to June 1993) of NOAA 11 data (version 6.0), reprocessed data are available from the Satellite Data Services Division (SDSD) of the NOAA National Environmental Satellite Data and Information Service (NESDIS) to study geophysical phenomena involving ozone. Although the archived data from the two spacecraft were processed using the similar science algorithms, there are significant differences in the long-term characteristics of the two data sets. These differences are the result of unique constraints and spacecraft environment. On NOAA 9 the onboard diffuser calibration system failed shortly after launch; therefore the archived data (version 5.0) have no diffuser calibration correction applied to them. In addition, the NOAA 9 data are not corrected for errors introduced by large fluctuation of the order of ±6°C in the photomultiplier tube (PMT) temperature resulting from the drift of the equator crossing time from 1430 to 1600. On the other hand, the NOAA 11 archived data (version 6.0) have been corrected for both PMT temperature variation and diffuser degradation. It is expected that the NOAA 9 deficiencies will be corrected in the next reprocessing of the data set.

The purpose of this paper is to identify and provide estimates of various sources of instrument errors and to determine their impact on columnar ozone measurements by the two instruments. The organization of this paper is as follows: Section 2 briefly describes the instrument and section 3 provides a detailed discussion of various sources of instrument errors and their impact on the albedo measurements (defined, in this paper, as the ratio of vertically emergent radiance to the incoming irradiance). Section 4 discusses the error in the retrieved ozone and section 5 contains results on the comparison with Dobson data. Summary and conclusions are given in section 6.

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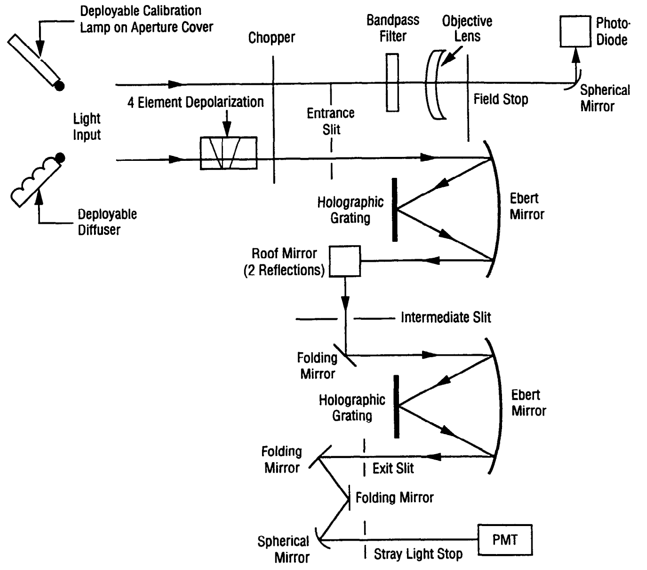

Figure 1. Schematic drawing of the solar backscattered ultraviolet (SBUV/2) instrument.

2. Instrument Description

Figure 1 shows a schematic of an SBUV/2 instrument. Details of the instrument and mode of operations can be found in the work of *Ball Aerospace Systems Division* [1981, hereinafter referred to as *BASD*] and *Frederick et al.* [1986]. Briefly, each SBUV/2 instrument consists of a tandem Ebert-Fastie double monochromator, a PMT detector, and a diffuser assembly. A separate narrowband filter photometer, called the cloud cover radiometer (CCR), is also located in the same structure assembly as the monochromator and it is coaligned with the monochromator's field of view. The CCR measures the Earth's surface brightness at 379 nm, where the ozone absorption is negligible. The purpose of the diffuser assembly is to enable the determination of the absolute solar irradiance at the top of the atmosphere. This is accomplished by reflecting the solar irradiance off an aluminum diffuser plate into the foreoptics of the instrument. The solar irradiance can be measured in either continuous or discrete scanning mode, as described below.

In the normal operational mode the SBUV/2 instrument measures backscattered ultraviolet radiation from the Earth's atmosphere at 12 discrete wavelengths, in the Hartley and Huggins bands of ozone, from 252.0 to 339.8 nm at 1.1-nm resolution. The field of view of the instrument is 11.3° × 11.3° which corresponds to a 200 km × 200 km instantaneous ground footprint for a nominal spacecraft altitude of 950 km. The instrument can also measure solar irradiance and backscattered atmospheric radiance in a continuous scan mode from 160 to 400 nm in nominal 0.148-nm increments. The instrument has three electronic gain ranges and can measure signals varying more than 6 orders of magnitude.

The SBUV/2 instruments on the NOAA 9 and NOAA 11 spacecraft differ from their predecessor SBUV instrument on the Nimbus 7 spacecraft in a few respects. Most importantly, the SBUV/2 instruments have the capability to monitor the relative reflectance of the diffuser plate in flight using a mercury (Hg) lamp onboard the calibration system. Also, the SBUV/2 instruments have onboard memory which can be programmed from the ground, so that the backscattered radiance and the incoming solar irradiance can be measured at wavelengths other than the 12 wavelengths used operationally for ozone retrieval. A comparison of some of the important features of SBUV/2 and SBUV instruments is given in Table 1.

Table 1. Comparison of Important Features of SBUV/2 and SBUV Instruments

Feature	SBUV/2	SBUV
Monochromator mode	4 (discrete, sweep, wavelength, and position)	4 (step, continuous, wavelength and cage cam)
Control of monochromator mode	2 (fix system and flex system (wavelengths can be changed by command after launch))	1 (fixed system)
Scene mode	4 (Earth, Sun, wavelength calibration, and diffuser check)	2 (Earth and Sun)
Diffuser position	4 (stow, Sun, wavelength calibration or diffuser check and diffuser decontamination)	3 (stow, Sun wavelength calibration)
Mercury lamp position	2 (stowed and deployed)	1
Cloud cover radiometer (CCR) wavelength	379 nm	343 nm
Shortest wavelength of discrete mode (other 11 wavelengths match)	251.9 nm (in fix system)	255.5 nm
Wavelength calibration steps	12	5
Electronic calibration	every scan in retrace	by command
Scanning		
discrete mode	32 s	32 s
sweep mode	192 s	112 s
Sampling time		
discrete	1.25 s	1 s
sweep	0.1 s	0.08 s
Diffuser check	yes	no
Diffuser decontamination	yes	no
Gain range	two ranges from PMT anode and one range from PMT cathode	three ranges from PMT anode; one range from reference diode
IFOV	11.3° × 11.3°	11.3° × 11.3°
Discrete (step scan) scanning direction	from short to long wavelengths	from long to short wavelengths

SBUV, solar backscattered ultraviolet. IFOV, instantaneous field of view. PMT, photomultiplier tube.

3. Instrument Performance

The primary quantity in the determination of ozone abundances from BUV-type observations is the ratio of the radiance from the Earth to the irradiance from the Sun, referred to here as the albedo, where ideally the only instrument element not common to both measurements is the diffuser used in the solar irradiance measurement. As a result, accurate knowledge of changes in diffuser reflectivity as a function of wavelength and time is required to significantly reduce the uncertainties in the calculation of long-term ozone trends. However, variations in the behavior of other instrument characteristics can also affect the accuracy of the derived ozone values in more subtle ways. For example, ozone observations made at high solar zenith angles are more likely to have signals which are output in electronic gain range 2, which is read from the PMT anode, whereas low solar zenith angle observations may have signals in range 3 which are read from the PMT cathode. Because the PMT anode output is a sensitive function of time, wavelength, and temperature, failure to accurately account for these effects will lead to incorrect ozone amounts in certain situations and to the introduction of nongeophysical effects into long-term trend calculations. Similar considerations apply to other instrument characteristics, such as wavelength calibration. Thus a thorough understanding of the changes in SBUV/2 instrument performance with time is essential in determining meaningful long-term trends in ozone.

The performance of each SBUV/2 instrument is characterized prior to launch with extensive end-to-end testing, including wavelength calibration, radiometric calibration, and goniometric calibration [*BASD*, 1985; *Frederick et al.*, 1986]. When in orbit, regular internal measurements are made to monitor the status of instrument electronics, wavelength calibration, and diffuser reflectivity [*Weiss et al.*, 1991, 1994; *Laamann and Cebula*, 1993]. By using carefully selected data sets from onboard observations, such as solar irradiance measurements, in conjunction with spacecraft engineering data, changes in instrument characteristics which are not directly monitored during flight, for example, the diffuser goniometric calibration, can also be determined. The following sections discuss some of the important instrument parameters which have been analyzed to study the impact of instrument performance on the accuracy of ozone retrieval from the NOAA 9 and NOAA 11 SBUV/2 instruments.

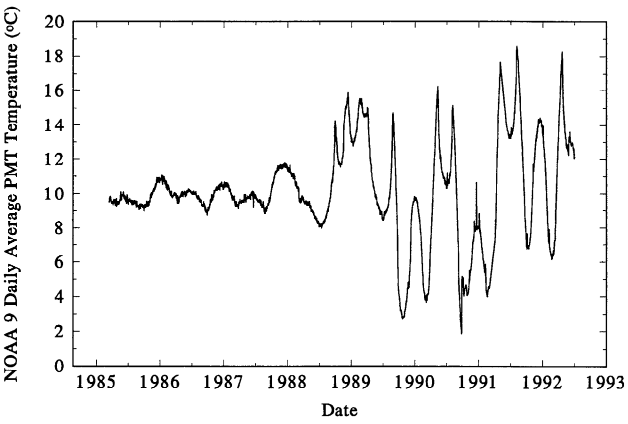

Figure 2a. Time series of the daily average NOAA 9 photomultiplier tube (PMT) temperature during solar irradiance measurements.

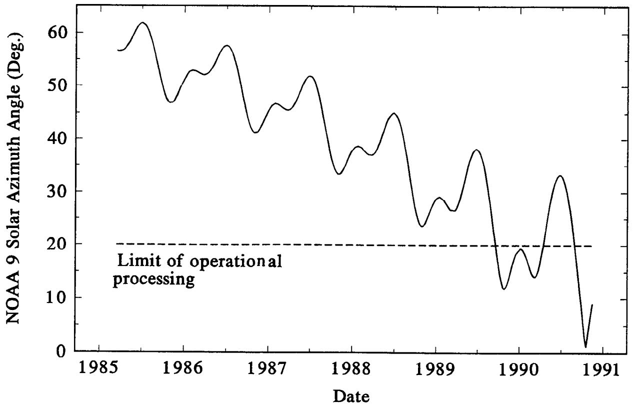

Figure 2b. Time series of the NOAA 9 solar azimuth angle for discrete mode solar irradiance measurements.

3.1. Radiometric Calibration

SBUV/2 absolute radiometric sensitivity is determined prior to launch for both radiance and irradiance measurements. Estimates of the 2σ absolute error in the albedo measurements based on the prelaunch calibrations for the NOAA 9 SBUV/2 are approximately 1.6% at 300 nm and 1.8% at 340–400 nm [*BASD*, 1981]. Propagation of these errors through the retrieval procedure described in section 4 leads to an estimated 2σ error of approximately 2.8% in the derived total ozone amount. Improvement of these error limits depends on quantities such as instrument noise and nonlinearity, differences in test equipment which do not cancel in the albedo determination, and errors in the calibration of the laboratory test diffuser. As previously mentioned for the in-flight measurements, diffuser errors are the primary source of uncertainty. Variations in other calibration-related parameters which can be monitored in space and which also impact instrument performance are described below.

3.1.1. PMT temperatures. Any measurement taken in electronic gain ranges 1 and 2 by the SBUV/2 instrument is read from the anode of the PMT, whose output is a function of temperature. The magnitude of the correction factor required for the PMT signal depends on the specific PMT itself and may be wavelength dependent in some cases but usually shows approximately a -0.2% change in signal for a 1°C change in the PMT temperature [*BASD*, 1985]. For the NOAA 9 SBUV/2 instrument the measured PMT temperature was stable to within ± 1°C during the first three years of operation but began to undergo large fluctuations as the spacecraft's orbit drifted to late afternoon equator-crossing times (see Figure 2a). This effect is illustrated by the time series of the NOAA 9 spacecraft-centered azimuth angle, β, in Figure 2b, where the initial value of $\beta \approx 57°$ represents a 1420 equator-crossing time and $\beta = 0°$ is a 1800/0600 orbit. The most extreme temperature fluctuations in August 1990 (see Figure 2a) are equivalent to a 3% variation in PMT output strength within a 1-month period. An algorithm to correct the PMT output for these temperature variations was derived by the SBUV/2 instrument manufacturer [*BASD*, 1985] but was not implemented in the NOAA 9 SBUV/2

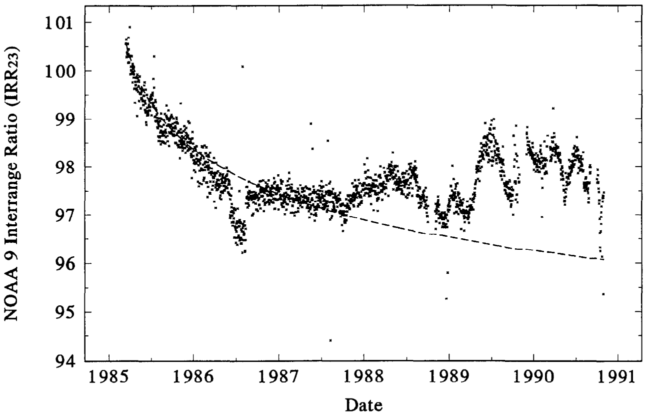

Figure 3a. Time series of the NOAA 9 gain range 2 to gain range 3 ratio ($IRR_{23}(t)$) from in-flight radiance measurements at 340 nm with a quadratic fit to 2 years of data (dashed curve).

version 5 data reprocessing. The algorithm provides a correction factor which corrects the PMT output to within 0.01% per °C change in temperature. This means that if the PMT temperature corrections are applied, the error in radiance/irradiance measurements will reduce to 0.1% or less. (Note that if the radiance and irradiance measurements are made on the same electronic gain range then the error will cancel out and there will be no error in the albedo.) In the absence of PMT temperature correction the NOAA 9 (version 5) albedo error varies from -0.2 to 0.2% from launch to September 1987 and from -1.2 to 1.4% afterward. Also, the magnitude of the NOAA 9 thermal variations, after fall 1988, may lead to second-order thermal effects in the SBUV/2 instrument, such as differential expansion of the instrument housing, which are not treated in the existing algorithm. Evidence for such effects has been seen by the shuttle SBUV/2 (SSBUV) instrument, which undergoes temperature changes of up to 20°C in 1 day in the shuttle environment [*Cebula and Hilsenrath*, 1992]. The NOAA 11 SBUV/2 instrument has experienced much less thermal variability than NOAA 9 (<1°C/month), with PMT output changes due to ΔT_{PMT} of less than 0.5% over 4 years at total ozone wavelengths. The PMT temperature variation is accounted for in the version 6 reprocessing of NOAA 11 data. As a result of the correction the radiance/irradiance error is <0.1%.

3.1.2. Interrange gain ratios. Because the SBUV/2 instrument records measurements in all three electronic gain ranges simultaneously, for certain levels of input signal the output from two gain ranges are both valid. These data can be used to monitor the behavior of the interrange ratio as a function of time and wavelength. The interrange ratio between gain ranges 1 and 2 (IRR_{12}) for both NOAA 9 and NOAA 11 is time invariant to better than ±0.2% and shows no wavelength dependence, which is consistent with the fact that both ranges are read from the PMT anode. The stability of $IRR_{12}(t)$ should therefore be comparable to the electronic calibration results discussed below in section 3.6, with little or no impact on total ozone. The interrange gain ratio between gain ranges 2 and 3 (IRR_{23}) has been observed to change as a function of both wavelength and time, and these variations must be properly characterized to ensure the accuracy of both radiance and irradiance measurements. Using two years of in-flight measurements, the interrange ratio time dependence $IRR_{23}(t)$ for the NOAA 9 SBUV/2 was characterized by a power law fit to within 1%, as shown in Figure 3a. However, the accuracy of this characterization after October 1987 is more difficult to assess due to large fluctuations in IRR_{23} at all wavelengths. Although the input data for the derivation of $IRR_{23}(t)$ have been corrected for PMT temperature variations (see section 3.1.1), the remaining fluctuations are still correlated with the thermal history shown in Figure 2a. This indicates the possibility of second-order thermal effects, such as differential instrument housing expansion, which will require further investigation. The wavelength dependence of IRR_{23} adopted for NOAA 9 (not shown here) is piece-wise linear, with a minimum at approximately 275 nm. The estimated albedo error due to the interrange gain ratio characterization is about 0.3% for the first 2 years, except for a brief period around June 1986 when it deviates from the power law by -1.3%. The error varies by about 1% during the third and the fourth year and by about 2% during the fifth and sixth year. For the NOAA 11 (version 6) reprocessing, the time dependence of IRR_{23} was characterized by a piece-wise polynomial function to incorporate the apparent instrument anomaly in September 1989 (see Figure 3b). The estimated albedo error due to the interrange gain ratio characterization of NOAA 11 is 0.2%. As with NOAA 9, the form of $IRR_{23}(\lambda)$ for NOAA 11 is approximately linear over the range of wavelengths used for ozone processing.

3.1.3. Offsets. Changes in the electronic offsets for each gain range over time could introduce a long-term trend in the derived ozone and solar irradiance values, the magnitude of which would vary depending on raw count levels at a given wavelength. Analysis of 5 years of NOAA 9 SBUV/2 data shows trends of ±1 count or less, which is below the resolution of each individual measurement. We estimate the corresponding error in albedo values for both NOAA 9 and NOAA 11 to be less than 0.1%.

3.2. Wavelength Calibration

The precise position of selected major emission lines in the spectrum of the onboard mercury calibration lamp are monitored regularly during in-flight operations to determine any long-term changes in the wavelength calibration of each SBUV/2 instrument. Analysis of the discrete mode wave-

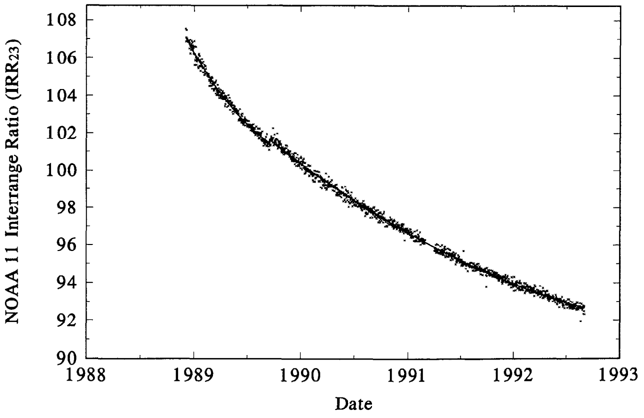

Figure 3b. Time series of NOAA 11 $IRR_{23}(t)$ at 340 nm with a piece-wise polynomial fit (solid curve).

length calibration measurements at 253.7 nm from NOAA 9 shows changes of the order of $\Delta\lambda \approx \pm 0.02$ nm during the first three years of operation (Figure 4a). Beginning in mid-1988, significant fluctuations are seen in the data. These fluctuations correlate with extreme variations in the NOAA 9 thermal history, as represented by the time series of the PMT temperature (see Figure 2a). As previously discussed in section 3.1.2, such fluctuations are probably indications of uncorrected thermal effects on the NOAA 9 SBUV/2 instrument. Confirmation that the large fluctuations are not caused by problems with the wavelength calibration system is provided by a similar analysis using the Mg II solar absorption feature at 280 nm, which gives comparable results [*DeLand et al.*, 1992].

For nominal observation conditions of 45° solar zenith angle and 325 Dobson units (DU) total ozone the estimated albedo error for the 312-nm channel is between ±0.3% from launch to fall of 1988 and then fluctuates between −0.3% and +0.7% in later years. The NOAA 11 SBUV/2 instrument has shown virtually no discernible wavelength scale drift during its first 3 years of operation, with $\Delta\lambda < 0.01$ nm based on mercury lamp measurements (see Figure 4b). This upper limit on wavelength scale drift corresponds to a maximum albedo error of 0.2% at 312 nm.

3.3. Mercury Lamp Stability

The SBUV/2 instruments incorporate a mercury vapor calibration lamp for tracking changes in diffuser reflectivity and wavelength calibration throughout the lifetime of the mission. A specific concern for the use of these lamps based on ground-based experiments was the stability of the lamp output, which directly affects any estimates of diffuser degradation. On the NOAA 9 SBUV/2 instrument, fluctuations of up to 20% in the mercury lamp output over intervals of a few days were observed beginning approximately one month after the start of regular operations [*Frederick et al.*, 1986]. This short-term instability in the lamp output rendered the onboard calibration system useless for determining diffuser reflectivity changes on NOAA 9. The onboard calibration system was redesigned for the NOAA 11 SBUV/2, with a substantial improvement in operational stability. The short-term output of the mercury lamp at 253.7 nm has remained stable to within ±1% during most of the first four years of operation on NOAA 11 [*Laamann and Cebula*, 1993]. Since the actual diffuser reflectivity variation used in the ozone derivation is a functional fit to the data, the random nature of the observed variations in lamp stability limits the possible diffuser reflectivity error to approximately 0.1% or less per year. The redesigned calibration system used for NOAA 11 has been implemented for each subsequent SBUV/2 instrument. For long-term use of the onboard calibration system the primary limiting factor is the availability of sufficient signal to make accurate measurements at all desired wavelengths. Although the absolute lamp output has decreased by approximately 45% in four years at 253.7 nm, the results obtained for NOAA 11 SBUV/2 suggest that the calibration measurements can be performed for at least 2–3 more years, given the existing level of stability [*Laamann and Cebula*, 1993].

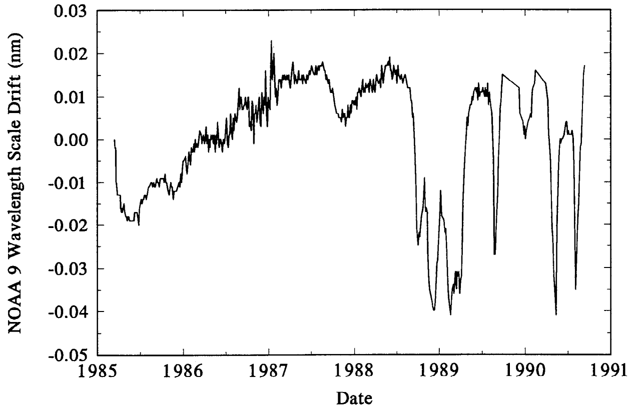

Figure 4a. Time series of the NOAA 9 discrete mode wavelength scale drift, as determined from the central position of the 253.7-nm emission line in the mercury calibration lamp spectrum.

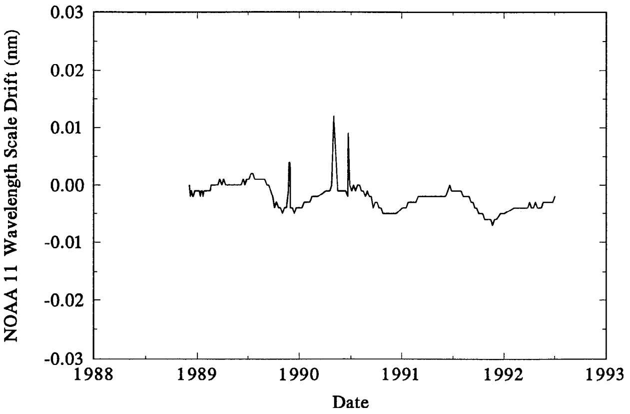

Figure 4b. Time series of the NOAA 11 discrete mode wavelength scale drift from mercury lamp measurements at 253.7 nm.

3.4. Diffuser Reflectivity

The SBUV/2 instruments are designed to monitor changes in diffuser reflectivity while in space by comparing the signal from a mercury lamp viewed directly with the lamp signal observed off the solar diffuser, thus isolating the instrument component not common to both radiance and irradiance measurements. As stated above, instabilities in the mercury lamp output began to appear after approximately 1 month of operation for NOAA 9, preventing the use of this system as designed [*Frederick et al.*, 1986]. However, the redesigned calibration system on NOAA 11 has proven successful. The most recent determination of the diffuser degradation wavelength dependence [*Laamann and Cebula*, 1993] shows that it can be characterized by a linear function (see Figure 5), with a 95% confidence limit on the calculated degradation rate of approximately ±0.1% per year based on the results from observation of the strongest lines in the Hg lamp spectrum. The linear regression fit gives values for the diffuser degradation of −0.7% per year at 340 nm, −0.8% per year at 331 nm, and −0.9% per year at 312 nm. The error in the observed albedos at the total ozone wavelengths due to incorrect determination of the diffuser degradation characterization is less than ±0.2% per year. However, if diffuser degradation correction is not available, as is the case with the NOAA 9 (version 5.0) reprocessing the albedo error (numerically equal to the diffuser degradation error) will increase with time. If we assume the NOAA 11 diffuser

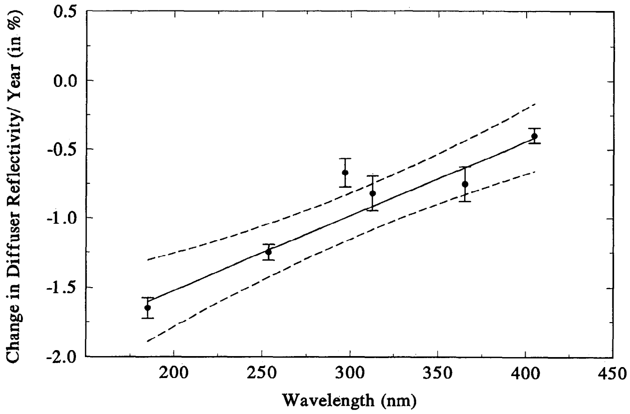

Figure 5. NOAA 11 diffuser reflectivity change rates derived from strong lines (circles) in the mercury calibration lamp spectrum, with $\pm 2\sigma$ error bars shown for each point. The solid line represents a weighted linear fit to the data, and the dashed curves denote the 95% confidence level of the fit. Adapted from *Laamann and Cebula* [1993].

degradation rate for NOAA 9, the corresponding albedo errors at 340, 331, and 312 nm at the end of October 1990 would be −4.2, −4.5, and −5.0%, respectively.

3.5. Goniometric Calibration

The goniometric calibration of an SBUV/2 instrument is a characterization of the scattering properties of the diffuser plate as a function of incidence angle. The calibration is performed as part of the prelaunch instrument test procedures and is intended to be valid within a specific range of angles representing the position of the solar ray with respect to the diffuser plate normal. Currently, a third-order Taylor series expansion in spacecraft-centered elevation and azimuth angles (α, β) is used to provide a smooth function for operational use. For the NOAA 9 SBUV/2 the prelaunch calibration has sufficed very well, with some possible errors at high azimuth angles during summer 1985 (see Figure 6). Because of the rapid drift of the NOAA 9 spacecraft orbit to later equator-crossing times, the solar azimuth angles measured by the SBUV/2 instrument fell below the prelaunch calibration limit of 30° in fall 1988, with longer periods of time affected in each succeeding year (see Figure 2b). In the current operational ozone production system for NOAA 9, discrete mode solar irradiance measurements are used in the production of albedo correction factors (ACFs), which provide a correction for changes in instrument behavior and solar activity. All solar irradiance measurements at $\beta > 20°$ are used in the current ACF derivation, while measurements taken at $\beta < 20°$ are rejected and replaced with interpolated values. Because large intervals of inaccurately interpolated ACFs could reduce the validity of any long-term trend results, it is important to reduce the need for such interpolation whenever possible.

Analysis of solar irradiance measurements taken at low azimuth angles ($\beta < 20°$) shows an increase in derived irradiance of up to 7% which is correlated with the decrease in azimuth angle, such as the fall-winter periods of 1989–1991 in Figure 6. In the range of azimuth angles used for operational ozone processing, the maximum irradiance error is less than 1%. The correlation between increased irradiance and observed azimuth angle suggests that a revised in-flight goniometric correction can be calculated from irradiance measurements which include the lower azimuth angles, thus reducing the length of time for which interpolation is necessary in the ACF time series. In the reprocessed NOAA 9 (version 5.0) ozone data, goniometric errors in the ACFs are avoided by using a functional fit to data taken in the region of valid goniometry as a representation of long-term instrument change at each wavelength [*DeLand*, 1991]. This approach reduces the albedo error to less than 0.9%. The NOAA 11 spacecraft was launched into an orbit with an earlier equator-crossing time than NOAA 9 but began to experience azimuth angle-correlated irradiance variations of 0.5–1.0% after 2 years of operation. An ACF derivation method similar to that used for NOAA 9 has been employed for the NOAA 11 (version 6.0) reprocessed data, and the estimated goniometric error in the diffuser measurements is less than 0.3% [*DeLand et al.*, 1993].

3.6. Electronic Calibration

After every sweep mode and discrete mode measurement scan by an SBUV/2 instrument, electronic calibration data are gathered as the grating drive resets to the starting position for the next scan. Analysis of electronic calibration data from the Nimbus 7 SBUV/TOMS instruments showed that the electronic systems were stable to ±0.1% [*Cebula et al.*, 1988]. This extensive volume of data has been only partially analyzed for both NOAA 9 and NOAA 11, but the available results indicate a similarly high degree of stability. Observed electronic subsystem changes for NOAA 9 SBUV/2 are no more than +0.5% during the first 2 years of operation, a significant portion of which may be attributed to a corresponding increase in the input reference voltage during that same period. We estimate the albedo error due to actual electronic calibration changes to be 0.1% or less. The NOAA 11 SBUV/2 reference voltage has been even more stable, with an increase of less than 0.1% in its first 2 years of operation. This is equivalent to an error in albedo of significantly less than 0.1%. Further analysis of these electronic calibration data will determine whether any significant long-term trends exist, but the impact on SBUV/2 instrument performance is clearly very small. The effect on derived ozone abundances is also estimated to be negligible.

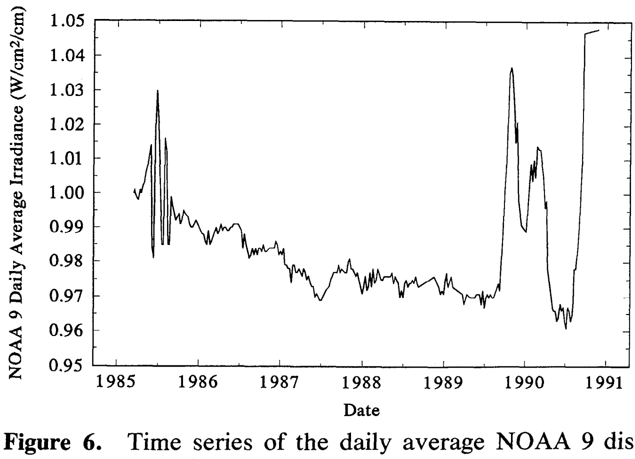

Figure 6. Time series of the daily average NOAA 9 discrete mode solar irradiance at 340 nm.

4. Impact on Ozone Estimation

The impact of instrument error on the accuracy of ozone retrievals can be estimated from the albedo errors (given in the preceding section) by propagating them through the ozone retrieval algorithm. The following paragraphs provide an overview of the ozone algorithm. The purpose of this overview is to provide the necessary background for discussing the ozone error resulting from various sources of instrument errors.

4.1. Ozone Algorithm

The SBUV/2 total ozone algorithm for NOAA 9 and NOAA 11 is based on a lookup table approach. The details of the algorithm can be found in the work of *Dave* [1978], *Klenk et al.* [1982], *NASA* [1990], and *NOAA* [1986]. Briefly, the lookup table contains computed nadir albedos for each wavelength of the ozone retrieval channels for 23 ozone profiles representing ozone distributions from the equator to the poles, 10 solar zenith angles, and two pressure levels. The ozone is computed from the N value, defined as $-100 \log_{10}$ of albedo. The reason for using the N value is that over a small range of ozone values (of the order of 50 DU) it is linearly proportional to the ozone amount. Also, total ozone is estimated from pairs of wavelengths rather than a single wavelength. The pairs are chosen in such a way that one wavelength is in the ozone absorption band and the other just outside the band. The main advantage of using a pair of wavelengths is that the ratio of the albedos of the pair is free from wavelength-independent errors. The algorithm uses three pairs, called the A, B, and C pairs. They are defined as (312 nm, 331 nm), (318 nm, 331 nm), and (331 nm, 340 nm), respectively. The best ozone value is derived from the pair ozone values as a weighted average by considering each pair's sensitivity to ozone for the optical pathlength of the observation.

The first step in the ozone retrieval is the determination of the effective reflectivity of the scene which is determined from the observed albedo at 340 nm. The next step is the calculation of the ozone, which is accomplished by an interpolation of the lookup table for the observed N value (for the pair) and solar zenith angle. In interpolating the lookup table, the algorithm assumes that the effective reflectivity is independent of wavelength. For solar zenith angles less than 70° the "best ozone" is essentially a weighted mean of A and B pair ozone values. At low and moderate solar zenith angles the values for the C pair are ignored because of the C pair's poor sensitivity to ozone. At high solar zenith angles the best ozone value is heavily biased toward B and C pair values, because the A pair ozone becomes very sensitive to the vertical distribution of ozone which is unknown.

4.2. Ozone Error

The albedo errors affect the total ozone estimate in two ways. One is through the error in the estimate of the effective reflectivity and the other is through the error in the ratio of the albedo of the pairs. Because effective reflectivity is derived from the 340-nm channel, only albedo errors for the 340-nm channel contribute to the ozone error from this source. For the purposes of error discussions we divide all instrument errors into two categories, systematic and random, and each category into wavelength-dependent and wavelength-independent errors. We note that for systematic errors in albedo which are wavelength-independent, the error in retrieved ozone comes primarily from the error in determining effective reflectivity. The error in the ratio of albedos cancels out. For random errors the error in retrieved ozone comes from both the reflectivity error and the error in the ratio of the albedos. Table 2 summarizes the ozone error estimates from each source. The table also identifies whether the error is systematic or random and whether it is wavelength dependent or wavelength independent. The ozone errors in Table 2 were computed using the following rule. A 1% increase in the 340-nm albedo (reflectivity channel) would result in 0.3% decrease in total ozone, whereas a 1% increase in the ratio of 312- to 331-nm albedos (A pair) would result in a 1% decrease in total ozone. These values refer to an atmosphere containing 325 DU of ozone, surface reflectivity of 20%, and solar zenith angle of 45°. For B and C pairs a 1% error in the ratio of albedos results in a 1.2 and 5% error, respectively, in total ozone. These values are for solar zenith angles of 75° and 85°, respectively. Unless otherwise stated, all ozone errors reported in this paper are for A pair ozone values.

In examining the various sources of errors, we find that for the NOAA 9 SBUV/2 instrument the dominant sources of errors are related to (1) large fluctuation in the spacecraft housing temperature and (2) the degradation in the diffuser reflectivity. For NOAA 11 SBUV/2 the dominant source of error is related to goniometric correction uncertainties caused by orbital drift. The large fluctuation in the NOAA 9 housing temperature was a result of the drift in the NOAA 9 orbit, as described in section 3.1.1. The large temperature

Table 2. Impact of Instrument Performance on Total Columnar Ozone

Quantity	Ozone Error,[a] % NOAA 9, Version 5.0	 NOAA 11, Version 6.0
Radiometric calibration (random; λ independent) (pre-launch)	±1.4	±1.4
PMT thermal calibration (systematic;[b] λ independent)	0.0[c,d]	0.0[c]
Interrange ratio ($IRR_{23}(t)$) (systematic;[b] λ independent)	0.0[c,d]	0.0[c]
Zero offsets/electronic offsets (systematic; λ independent)	0.0[c]	0.0[c]
Wavelength calibration (systematic;[b] λ dependent)	−0.4[e]	0.0[c]
Diffuser reflectivity (systematic;[b] λ dependent)	−1.9[e,f]	−0.3[g]
Goniometric calibration (systematic;[b] λ independent)	−0.3[e]	−0.1[g]
Electronic calibration (systematic; λ independent)	0.0[c]	0.0[c]
Total ozone error (postlaunch)	−2.6[e] (−2.2)[h]	−0.4[g]

[a] All errors quoted in this table are 1σ errors. Also, errors have been rounded off to one place after decimal.

[b] Time-dependent systematic error.

[c] Error is less than 0.1%.

[d] When the pair wavelengths are sampled on the same electronic gain range. Generally valid for all observations with solar zenith angle less than 60°.

[e] At the end of October 1990.

[f] Based on the degradation rate experienced on NOAA 11.

[g] At the end of June 1993.

[h] Based on the trend after June 1989.

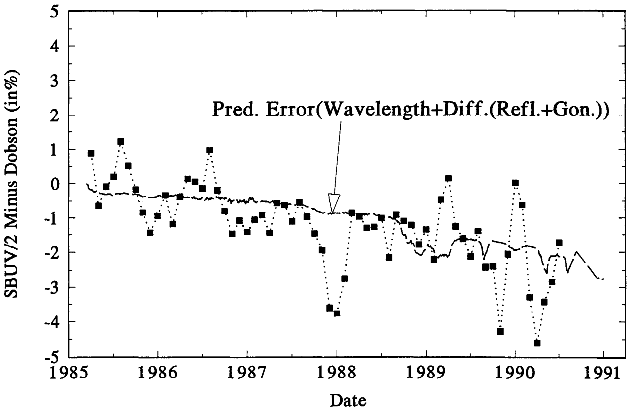

Figure 7. Time series of postlaunch NOAA 9 SBUV/2 instrument error (dashed curve) and of the difference of coincident ozone measurements from NOAA 9 SBUV/2 and Dobson instruments (dotted curve with squares).

fluctuation after 1988 significantly impacted the PMT throughput, the interrange ratio, and the wavelength calibration. For example, during August 1990 the PMT temperature fluctuated from 15°C to 2°C (see Figure 2a), whereas the nominal operating temperature during the first 3 years was 10 ± 1°C. From the temperature sensitivity discussion in section 3.1.1 we find that a change of −8°C would introduce a 1.6% change (decrease) in albedo when the Earth radiances are measured on either gain range 1 or gain range 2 and the irradiance is measured on gain range 3. If this variation is assumed to be independent of wavelength, the maximum ozone error (increase) would be 0.5%. This error is a result of the error in the effective reflectivity. Fortunately, most of the 340-nm radiance data ($\theta_0 < 87°$) are on gain range 3; therefore they are not affected by this source of error.

For NOAA 9 the effect of interrange ratio (IRR_{23}) error propagates through the ozone algorithm in a somewhat complicated manner. The reason for this is that a power law is used to characterize the time-dependent behavior of IRR_{23}. Because the interrange error affects both the radiance and the irradiance measurements, the error in the albedo measurement cancels out if the radiance and the irradiance measurements of ozone wavelengths are taken on the same gain range. An examination of the irradiance and radiance measurements and corresponding gain ranges show that all irradiance measurements (at total ozone wavelengths) are taken on gain range 3 and most of the radiance measurements, generally up to 60° solar zenith angles (small optical pathlength), are also taken on gain range 3. In other words, for most of the albedo measurements the interrange ratio error is essentially zero. When the optical pathlength increases, the error first appears in the *A* pair ozone and then in the *B* pair ozone values. An examination of the solar zenith angle measurement distribution suggests that the impact of the interrange ratio error is large at high latitudes, particularly in the later years, when due to orbital drift, most of the measurements are taken at high solar zenith angles. For example, after March 1989 the ozone error is as high as 2%.

As noted in section 3.2, the large fluctuation in the housing temperature also affected the wavelength calibration. We find that from the launch to the fall of 1988, $\Delta\lambda$ is about ±0.2Å (see Figure 4a), which introduces an ozone error of about ∓0.2%. After the fall of 1988, $\Delta\lambda$ varies between −0.4Å and +0.2Å. This produces an ozone error which varies between +0.2% and −0.4%.

For NOAA 11 the PMT operating temperature and wavelength calibration are very stable. We estimate the ozone errors from each of the two sources to be 0.03%. Also, the power law provides a good description of the time-dependent behavior of IRR_{23}, and the ozone error at high optical pathlength is estimated to be less than 0.1%.

The ozone error due to a zero offset is very small. We estimate it to be about 0.03% for both NOAA 9 and NOAA 11. With regard to the diffuser degradation error the onboard calibration system for NOAA 9 failed shortly after launch, and therefore we do not have any direct quantitative information regarding changes in diffuser reflectivity with time. However, we can estimate the magnitude of the NOAA 9 diffuser plate degradation from the time history of the NOAA 11 diffuser plate because the two diffuser plates were made of the same material. Assuming NOAA 11 degradation rates, the NOAA 9 diffuser error, at the end of October 1990, would be −1.9%. For NOAA 11 the ozone error due to uncertainty in the diffuser plate characterization is 0.3%.

Based on the albedo errors given in section 3.5, we estimate that the goniometric calibration error for NOAA 9 and NOAA 11 are −0.3 and −0.1%, respectively. We note that of all the errors, the diffuser-related errors (reflectivity and goniometry) contribute most to the uncertainty in determining the trend in ozone abundance.

In summary, for NOAA 9 (version 5.0) the total postlaunch error in columnar ozone at the end of the data record (October 31, 1990) is −2.2%. In computing this error, we added the contributions of the wavelength, diffuser reflectivity, and goniometric error estimates listed in Table 2. This error estimate applies to all observations with solar zenith angles less than 60°. For a solar zenith angle greater than 60°, the error increases because of the incorrect characterization of the interrange ratio IRR_{23}. For NOAA 11 (version 6.0) the total postlaunch error at the end of its data record (June 1993) is less than −0.4%. The time-dependent history of the postlaunch error is discussed in the following sections.

5. Comparisons With Dobson Data

As part of the overall evaluation of the SBUV/2 total ozone data, *Planet et al.* [1994] have compared NOAA 11 (version 6.0) total ozone data with those available from Dobson spectrophotometer data obtained from the World Ozone Data Center in Toronto. Here, we report additional results on comparison with NOAA 9 (version 5.0) and Dobson data. The method of creating match-up data set is similar to those described by *Planet et al.* [1994].

Figure 7 presents the results of the comparison of NOAA 9 and Dobson data. All of the Dobson data in the comparisons either used the *Bass and Paur* [1984] ozone absorption coefficients or were adjusted from the previous values so that they would be compatible with the Bass and Paur coefficients. (The old values were derived using the Vigroux coefficients [*Vigroux*, 1953]). Figure 7 also shows the total estimated postlaunch error (consisting of the wavelength, diffuser reflectivity, and goniometric errors) as a function of time. An examination of Figure 7 shows that the NOAA 9 data trend downward with respect to the Dobson observations by about 2.5% over the 5.5 years of the data record.

This is consistent with results derived solely on the basis of detailed error analysis. We also note that from 1989 onward, the variability of the NOAA 9 comparisons increased considerably. This result is probably due to the spacecraft's orbital characteristics in the later years, which limits the availability of the useful data and reduces the number of stations with at least five match-ups per month to considerably less than 30. From the error discussion in the preceding section we find that about −1.9% of the trend can be attributed to the diffuser plate and most of the remaining −0.6% to some combination of wavelength calibration error, interrange ratio error, goniometry, the match-up statistics, and error in the Dobson measurements. For NOAA 11, *Planet et al.* [1994] did not find any significant divergence with respect to the Dobson observations.

6. Summary and Conclusion

In this paper we described in detail various instrument errors that affect the accuracy of total ozone estimates from the SBUV/2 instruments on the NOAA 9 and NOAA 11 spacecraft. We reported that soon after the launch of NOAA 9, the mercury lamp in the SBUV/2 housing failed and the instrument lost all of its onboard diffuser plate calibration capabilities. The onboard calibration system on NOAA 11, however, is still working satisfactorily and the diffuser plate has retained its reflective properties fairly well. Over a 4-year period it has degraded by about 2.9% at 400 nm and about 3.5% at 312.5 nm. This degradation has been accounted for in the version 6.0 processing of NOAA 11 data. The residual error due to uncertainty in the characterization of the diffuser degradation is estimated to be −0.3%. Also, if we assume the NOAA 9 diffuser degradation rate is similar to the NOAA 11 degradation rate, the diffuser-related ozone error at the end of the NOAA 9 data record (October 1990) would be about −1.9%. We note that of all the errors discussed in this paper, the diffuser errors contribute most to the uncertainty in determining the trend in ozone from SBUV/2 instrument.

In our analysis we also observed that the equator-crossing time for NOAA 9 was not constant but smoothly changed with time. Initially, in 1985 it was 1430, but by January 1990 it became 1730. This change resulted in a large seasonal variation in the spacecraft's temperature which affected the performance of the instrument. In particular, the PMT throughput showed large changes which at times were as high as 3%. The large PMT variation also affected the ozone estimates. However, we believe that when proper temperature corrections are applied in a future reprocessing, the PMT throughput would come more in line with the operational specification. Our analysis shows that after the PMT temperature corrections are applied, the residual PMT error is less than 0.1% in the albedo measurement for both NOAA 9 and NOAA 11.

The drift in the NOAA 9 orbit also caused the solar rays to fall on the diffuser plate at azimuth angles outside the range of goniometric calibration. Our analysis shows that for the range of azimuth angles used for operational processing (including the extrapolated angles), the maximum irradiance error due to goniometric calibration uncertainties is less than 1%. If we assume the error to be wavelength independent, then the corresponding error in ozone would be less than 0.3%. We estimate the NOAA 11 goniometric calibration error transferred to ozone error to be less than 0.1%.

With regard to wavelength calibration we observe that during the first 3 years of operation, NOAA 9 wavelength calibration at 253.7 nm (the strong Hg line) drifted by about ±0.02 nm. Beginning in 1988, it showed periodic large fluctuations which were found to be highly correlated with the large temperature changes in the spacecraft environment caused by the drift of the NOAA 9 orbit. The impact of wavelength drift on the ozone estimate was determined by examining the changes in the ozone absorption coefficients as a function of wavelength. In the version 5.0 reprocessing of NOAA 9 data, the effect of the large fluctuation in wavelength calibration is not accounted for. We estimate the ozone error after 1989 from this source to vary from +0.2 to −0.4%. NOAA 11 has not shown any discernible wavelength drift during the first 3 years of operation. We estimate the maximum error for NOAA 11 to be less than 0.03%.

Also, a comparison with a selected number of coincident Dobson stations, where the Dobson data were recently adjusted using Bass and Paur absorption coefficients, shows that NOAA 9 data drift downward by about 2.5% over a 5.5-year period. This result is consistent with the error estimate (−2.2%) derived from detailed error analysis. For NOAA 11, *Planet et al.* [1994] do not report any significant trend relative to coincident Dobson data.

In summary, the measurements from the SBUV/2 instrument on NOAA 11 are more stable than those from NOAA 9 SBUV/2, specifically due to reduced orbital precession effects and an accurate characterization of diffuser reflectivity change. Also, we believe that when the effect of the temperature and diffuser-related errors for NOAA 9 are accounted for, the total instrument-related error on the ozone retrieval from the two instruments will be very similar.

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