Version 8 SBUV Data - Documentation

A. Profile Screening

The Version 8 (V8) SBUV algorithm applies a number of quality control tests to each profile ozone measurement during processing. The results of these tests are summarized in the profile error flag listed in each compressed data record. An additional measure of data quality is provided by the average final residual value for each profile. The final residual at each wavelength represents the difference between the predicted radiance (calculated using the solution ozone profile) and the observed radiance. All final residual values for each profile are combined into a residual quality control parameter (ResQC) that can be used to select data for further analysis, as described in Section B.

B. Data Selection Suggestions

The V8 SBUV profile ozone data records contain flags that can be used to select specific types of data for analysis. This brief description provides suggestions on how to use the profile error flag and residual quality control flag (ResQC). The profile error flag has three components: the value in the ones place indicates the profile error code, the value in the tens place indicates an ascending [=0] or descending [=1] orbit measurement, and the value in the hundreds place indicates the validation code. A complete description of the profile error code and validation code are given in Sections C and D, respectively.

1. Initial data analysis should only use data with a profile error flag of 0. This selects ascending orbit measurements with the profile error code and validation code equal to 0, and a maximum solar zenith angle of 84°. These data have a maximum ResQC value of 0.20. For any individual instrument, a lower ResQC limit can be chosen at the cost of reducing data coverage. A time history of monthly ResQC flag values for equatorial ozone measurements is shown in Figure 1. Additional coverage during summer months at high latitudes can be obtained by accepting descending orbit measurements (profile error flag = 10) to ensure that all profiles up to solar zenith angle = 84° are available.

2. ResQC values greater than 0.20 may indicate either an instrument measurement error for that scan and/or an atmospheric effect not accounted for by the V8 ozone algorithm. To analyze data with ResQC values greater than 0.2, the user should include measurements with a profile error code of 3 (*e.g.* profile error flag = 3, 13). An additional filter for specific ResQC limits can be added, based on user analysis requirements. Further information about high ResQC scans is available in the complete level 2 data record.

3. Restricting data selection to profile error flags less than 100 (validation code = 0) will leave gaps in the overall time period represented by the V8 data (November 1978 to December 2003). If a complete time series is desired, the user should also include data with validation code = 1. This corresponds to selecting profile error flag = 100 for ascending orbit measurements (Nim-

bus-7, NOAA-9 1986-1989, NOAA-11 1988-1995, NOAA-16), and profile error flag = 110 for descending orbit measurements (NOAA-9 1993-1997, NOAA-11 1997-2001).

4. Increased coverage at high latitudes can be obtained by including data with a profile error code of 1 (solar zenith angles = 84°-88°). This corresponds to profile error flags = 1, 101 for ascending orbit data, and profile error flags = 11, 111 for descending orbit data.

5. Data selection may be further expanded by including profile error codes of 2, 4, and 5. The user should be aware that these codes generally indicate significant anomalies in the profile retrieval, and analysis results including such data should be evaluated with caution.

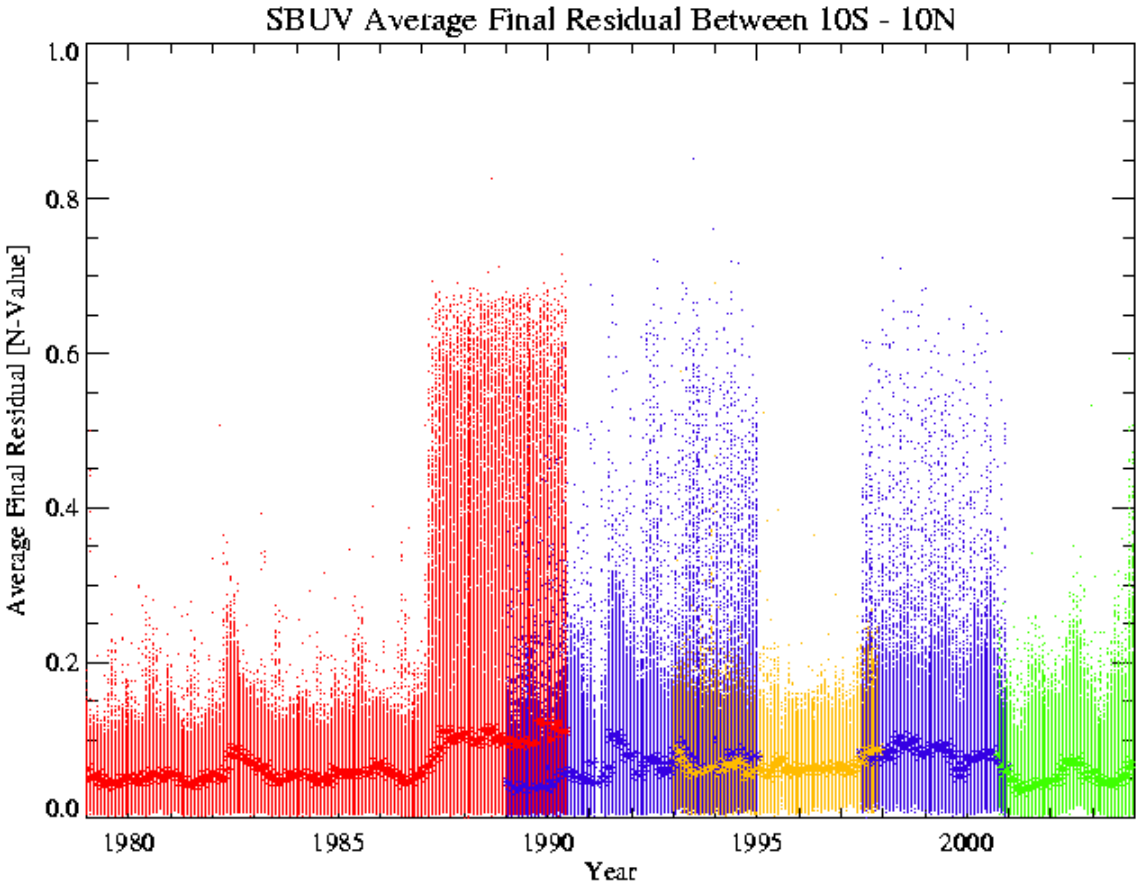

Figure 1. Time history of final residual quality control (ResQC) flag for different SBUV instruments. Asterisks represent monthly averages. *red*=Nimbus-7 SBUV, *gold*=NOAA-9 SBUV/2 (descending orbit), *blue*=NOAA-11 SBUV/2, *green*=NOAA-16 SBUV/2. The NOAA-9 ascending orbit data for 1986-1989 are not shown for clarity, but have similar ResQC values to the NOAA-9 descending orbit data.

C. V8 Profile Error Code

This section describes all profile error code values created by the Version 8 algorithm. Please note that only profiles with error codes = 0-5 are included on this DVD. If more than one value

among error codes 2-9 can be applied to a profile, the highest value is used. A summary list is presented first, followed by a more detailed description of each code value.

0 – Good retrieval.
1 – Solar zenith angle > 84°.
2 – abs[Step 3 total ozone – Profile total ozone] > 25 D.U.
3 – Average abs[final residue] > 0.20 N-value.
4 – abs[Final residue] > (3 * instrument error).
5 – abs[Retrieved – A Priori] > (3 * *a priori* error).
6 – Non-convergent solution.
7 – Upper level profile anomaly.
8 – Initial residue greater than 18.0 N-value units.
9 – Total ozone algorithm failure: first guess not available.

10 is added to the error flag value to indicate data taken in descending mode.
100 is added to the error flag value to indicate a broad period of lesser quality data (see discussion in Section D).

Definitions

0. No problems or anomalies in the profile retrieval.
1. The profile retrieval may have increased uncertainty at high SZA. Note that if this flag is set, the tests for error codes 2-5 are not applied.
2. The V8 algorithm calculates total ozone values using two methods: a TOMS-type retrieval (Step 3), and by summing all layers in the ozone profile (Profile). If the difference between these results exceeds 25 Dobson units, the error code is set to 2.
3. The final residue is calculated for each wavelength used in the profile retrieval and expressed in terms of N-value, where $N_\lambda = -100\log_{10}(I_\lambda/F_\lambda)$. We use the absolute value of each final residue and calculate the average to create the residual quality control flag (ResQC) for each profile. If ResQC is greater than 0.20, the error code is set to 3.
4. If the final residue at any wavelength is greater than 3 times the specified instrument error (currently 1.0%), the error code is set to 4.
5. If the difference between the retrieved ozone profile and the *a priori* ozone profile in any layer is greater than 3 times the specified a priori error (currently 50%), the error code is set to 5. This code value is intended to identify anomalous behavior in the lowest profile layers, where SBUV/2 data have very little information content.
6. If the profile algorithm fails to converge on a solution after 8 iterations, the error code is set to 6.
7. If the solution profile above 1 hPa deviates significantly from an exponential altitude dependence, the error code is set to 7.
8. For profiles with very large residue values, the error code is set to 8.
9. If the total ozone algorithm retrieval is unsuccessful, no profile retrieval is attempted, and the error code is set to 9.

D. Validation Code

A validation code of 100 is added to the V8 profile error flag to indicate periods where we have less confidence in the profile ozone data, based on internal validation results. This code frequently represents instrument performance problems. In most cases, the best available correction for the problem has been applied to the data, but residual errors may still be present. The quality of both total ozone and profile ozone data are affected. Small jumps of 1-2% in total ozone and 5-10% in profile ozone may be observed. Due to the increased noise during such periods, we are unable to identify every perturbed profile with an error flag. Please view unusual profiles during these periods with some skepticism. The validation code is also used to indicate periods where ozone data show greater differences in limited latitude and/or altitude regions, such as the first half of the NOAA-9 data record. The following text gives further descriptions of the periods for which this code has been assigned.

Validation Code Data Periods

Nimbus-7 SBUV Non-Sync [*February 1987 – June 1990*]
The Nimbus-7 SBUV chopper wheel began to lose synchronization with the counting electronics on February 13, 1987. Measurements made after this date were characterized by significantly higher noise in each scan. A correction function was developed based on the coherence of coincident 343 nm photometer data, as described by *Gleason and McPeters* [1995]. This correction decreased monthly average Umkehr layer ozone standard deviation values by 20-50%. Nimbus-7 profile ozone data during the "non-sync" period (1987-1990) do not show a bias relative to the 1978-1986 data. However, anomalous profiles are much more likely to occur during this period, and users should be cautious when examining individual ozone profiles. Approximately 15% of the Nimbus-7 profiles during the non-sync period have ResQC values greater than 0.2.

NOAA-9 SBUV/2 Terminator Crossing [*Fall 1990*]
The orbit of the NOAA-9 spacecraft drifted significantly during its lifetime, crossing through the terminator (1800/0600 UT Equator-crossing time) in September 1990. NOAA-9 SBUV/2 ozone measurements were made on the ascending node of the orbit (afternoon Equator-crossing time) from February 1985 to September 1990, and on the descending node (morning Equator-crossing time) from September 1990 to February 1998. Comparisons between NOAA-9 zonal average profile ozone and external data sets (sondes, Umkehr measurements) indicate step changes of 5-10% in NOAA-9 ozone values at some latitudes and upper levels between ascending node and descending node data. The NOAA-9 inter-instrument offset was adjusted based on comparisons between NOAA-9 and NOAA-11 in 1993, when both instruments observed at similar solar zenith angles. As a result of this adjustment, NOAA-9 ascending data are offset relative to other data sets. No change in instrument performance has been identified as a cause for this result. The NOAA-9 ascending node data for July 1986 to June 1989 are included separately on this DVD to provide an alternate source of ozone profiles during the Nimbus-7 SBUV non-sync period. These NOAA-9 data should not be used in long-term trend analysis unless absolute adjustments are applied. The NOAA-11 satellite orbit also crossed the terminator, but NOAA-11 profile ozone data do not show a step change between March 1995 (end of ascending node measurements) and July 1997 (first descending node measurements).

SBUV/2 Grating Drive [NOAA-9: *October 1993 – February 1998*; NOAA-11: *September 1993 – March 1995, July 1997 – March 2001*]

During the later part of the NOAA-9 and NOAA-11 SBUV/2 operating lifetimes, each instrument's grating drive began to experience wavelength selection problems. Errors up to three grating positions (1 grating position = 0.075 nm) were observed for some channels and time periods. The albedo values have been corrected for the indicated wavelength selection errors using nominal ozone cross-section and solar irradiance spectra. The actual wavelength for a sample may still be in error by up to 0.038 nm because of digitization in the grating drive readout. These wavelength errors produce increased errors in the profile ozone data.

NOAA-16 SBUV/2 Signal Spikes [*March 2001 – December 2003*]
The NOAA-16 SBUV/2 instrument experiences periodic negative data fluctuations ("spikes") due to electronic interference from another instrument on the NOAA-16 spacecraft. These spikes are primarily observed at 331.2 nm and 339.8 nm, and lead to erroneous derived surface reflectivity and aerosol index values, which impacts the derived total ozone value. Many of the affected measurements have been identified and assigned a V8 total ozone error flag value of 1. These data represent up to 10% of the NOAA-16 total ozone observations for a single day, beginning in March 2001. The intensity of the problem varies with time, and very few measurements are flagged in some months.