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User's Guide for the Solar Backscattered Ultraviolet (SBUV) Instrument First-Year Ozone-S Data Set

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PREFACE

NIMBUS EXPERIMENT TEAM (NET) VALIDATION STATEMENT FOR FIRST YEAR SBUV/TOMS OZONE DATA SET

Total ozone and ozone vertical profile results for Solar Backscattered Ultraviolet/Total Ozone Mapping Spectrometer (SBUV/TOMS) operation from November 1978 to November 1979 are available. The algorithms used have been thoroughly tested; the instrument performance examined in detail; and the ozone results have been compared with Dobson, Umkehr, balloon, and rocket observations. The accuracy and precision of the satellite ozone data is good to at least within the ability of the ground truth to check and is self consistent to within the specifications of the instrument.

The primary input to the ozone retrieval algorithms is the ratio of the backscattered radiance to the incident solar radiance. Both radiance and irradiance are measured separately by the SBUV and TOMS instruments. Accuracy in the determination of this ratio depends upon the calibration accuracy of a diffuse reflector used to measure the solar irradiance. Precision in the measurement of this ratio is better than 0.5% for SBUV and 1.0% for TOMS. Prelaunch calibration uncertainties affect the absolute accuracy of these measurements. We are continuing to assess the magnitude of these uncertainties. During the first year of instrument operation inflight diffuser degradation is less than 1.5% at 339.8 nm and less than 3.0% at 273.5 nm. No correction for this has been applied to the data. This inflight degradation can introduce an apparent long term drift in an analysis of the data.

One of the major design improvements of the Nimbus 7 SBUV instrument over the BUV instrument on Nimbus 4 involved the employment of a system for the on-board subtraction of dark current. This has improved the instrument's performance to a point where no radiation induced signal has been observed in the South Atlantic anomaly to date.

Total ozone has been derived from both the SBUV and TOMS instruments. Analysis of the variance of comparisons between colocated TOMS and AD pair direct sun (00 code) Dobson observations shows that total ozone retrieval precision is better than 2% to within 10 degrees of the solar terminator. There are biases of -6.5% and -8.3% for TOMS and SBUV respectively when compared to the Dobson network. These biases are primarily due to inconsistancies in the ozone absorption coefficients used by the space and ground systems. If absorption coefficients available on a preliminary basis from the National Bureau of Standards were used for both SBUV/TOMS and the Dobson measurements, the biases would be less than 3%.

Vertical profiles of ozone have been derived from the SBUV step scan radiances at 273.5 nm and longer wavelengths using an optimum statistical inversion algorithm. Comparison with Umkehr measurements at Boulder and Arosa indicate that the precision of the derived layer ozone amounts is on the order of 5%.

The altitude range, for which the inferred SBUV profiles is determined primarily by the radiance measurements, depends on several factors including the solar zenith angle, the total ozone amount, and the shape of the ozone profile. This altitude range typically extends from 0.7 mbar (50 km) down to the peak of the ozone density profile (20-40 mb) or 22-26 km.The derived layer ozone amounts below this region as produced by the optimum statistical inversion algorithm depend on the a priori statistical information about the correlation between these layers and the observed total ozone and upper level profile amounts.

Variations of UV solar flux associated with the rotation of active regions on the sun (27-day solar rotation period) have been observed with the continuous scan solar observations (160-400 nm). However, no significant solar flux variation was observed at the wavelengths used for the total ozone and vertical profile retrievals. Therefore, a long term smoothed solar flux was used in the processing with no 27 day period component. To the extent that there may have actually been a small 27 day period in the real solar flux this would introduce a small (less than 1/2%) artifact in the data.

Ground truth for the SBUV ozone profile consists of Umkehr profiles, ozone balloon sondes, several optical ozone rocket sondes, and a chemiluminescent rocket sonde. This set of data was not sufficient to precisely determine the accuracy and validity range of the satellite retrievals or to evaluate possible latitudinal or temporal trends in the data. However, there are indications that the SBUV values may be slightly (5%) lower than the balloon and Umkehr measurements below the mixing ratio peak (5-7 mb). At upper levels the agreement with the optical ozonesonde rockets flown in November of 1979 for the International Ozone Rocket Intercomparison is within ± 5%.

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CONTENTS

Section Page

1. SOLAR BACKSCATTERED ULTRAVIOLET EXPERIMENT 1

    1.1 Introduction 1
    1.2 Instrument Overview 2
    1.3 Theoretical Foundations 3

2. THE ALGORITHM 6

    2.1 Total-Ozone Algorithm 6

        2.1.1 Computation of Theoretical Radiances . . . 6
        2.1.2 Computation of Normalized Radiances (I/F) . 7
        2.1.3 Calculation of Reflectivity 10
        2.1.4 Calculation of Total Ozone 10
        2.1.5 Calculation of IFOV Pressure 12
        2.1.6 Calculation of Best Ozone 14
        2.1.7 Validity Checks 15

    2.2 Profile Algorithm 18

        2.2.1 Inversion to Obtain Profile 18
        2.2.2 Calculation of Multiple-Scattering Component 19
        2.2.3 *A Priori* Profile and Covariance Matrix . . 20
        2.2.4 Measurement Covariance Matrix 24
        2.2.5 Validity Checks 24

3. TAPE FORMATS 26

    3.1 Physical Structure of Ozone-S Tape 26
    3.2 Logical Structure of Tape 28

REFERENCES 52

APPENDIX A--F_2' CORRECTION FUNCTION 55

APPENDIX B--SAMPLE FORTRAN PROGRAM AND JCL FOR THE OZONE-S TAPE 59

APPENDIX C--DATA AVAILABILITY AND COST 63

APPENDIX D--SBUV OZONE-S TAPE CATALOG 65

ILLUSTRATIONS

Figure		Page
1	Quality Flags	16
2	Block Identifier	28

TABLES

Table		Page
1	External Inputs	8
2	*A Priori* Profile Coefficients	22
3	*A Priori* Profile Error Covariance Matrix	23
4	Format of First Record on Data Files	30
5	Data Record Format for OZONE-S Tape	33
6	Format of Last Record on Data Files	45
7	Format of Trailer File Record	48

USER'S GUIDE FOR THE
SOLAR BACKSCATTERED ULTRAVIOLET (SBUV) INSTRUMENT
FIRST-YEAR OZONE-S DATA SET

1. SOLAR BACKSCATTERED ULTRAVIOLET EXPERIMENT

1.1 INTRODUCTION

The solar backscattered ultraviolet (SBUV) instrument was proposed by D. F. Heath for Nimbus-G (7), and it represents an improved version of the backscattered ultraviolet (BUV) instrument that was proposed by D. F. Heath and J. V. Dave and flown on Nimbus 4. The instrument design is described by Heath *et al.*[1] The principal improvements incorporated into the Nimbus 7 SBUV instrument were: (1) mechanical chopping of the electromagnetic radiation entering the entrance slit of the double monochromator, which eliminated all interference from high-energy trapped-particle radiation; (2) stowing the solar-viewing diffuser plate except when observing the Sun in order to reduce the effects of spacecraft outgassing contaminants; and (3) the incorporation of a continuous scan (0.2-nm intervals) mode for observing either the Sun or the Earth in the 160- to 400-nm wavelength regions.

The combined SBUV/TOMS instrument has been supported by an experiment team consisting of D. F. Heath, Chairman, A. J. Krueger, C. L. Mateer, A. J. Miller, D. Cunnold, A. E. Green, A. Belmont, and W. L. Imhof. The SBUV/TOMS instrument was built by Beckman Instruments, Inc., of Anaheim, California. Algorithm development, evaluation of instrument performance, ground-truth validation, and data production efforts were carried out by A. J. Fleig, K. F. Klenk, P. K. Bhartia, H. W. Park, K. D. Lee, and V. G. Kaveeshwar of the Ozone Processing Team (OPT). The OPT is managed by A. J. Fleig and is supported by individuals from Systems and Applied Sciences Corporation and Goddard Space Flight Center.

This guide is intended for the users of the Nimbus 7 SBUV first-year total-ozone and ozone profile data set. This section describes the SBUV instrument and the theoretical foundations behind the experiment. Section 2 presents the algorithm used to produce the total-ozone and profile data sets and lists external information pertinent to the retrieval algorithm (namely, the absorption and scattering coefficients and the solar flux at each of the SBUV wavelengths). For a more detailed account of the theory behind the algorithm, see Klenk et al.[2] and references therein. Section 3 describes the ozone tape formats. Appendix A contains the correction functions used for obtaining the albedos. Appendix B contains a sample Fortran program and job control language (JCL) that can be used for reading an SBUV ozone tape. Appendix C contains information on ordering tapes. Appendix D contains a catalog of available tapes.

1.2 INSTRUMENT OVERVIEW

The SBUV instrument that is on board the Nimbus 7 satellite is designed to measure the total ozone and its distribution with height in the atmosphere in a vertical column beneath the satellite. The SBUV contains a double monochromator and a filter photometer designed to measure ultraviolet (UV) spectral intensities. In its primary mode of operation, the monochromator measures solar radiation backscattered by the atmosphere in 12 wavelength bands in the near-UV, ranging from 255.5 to 339.8 nm, each with a bandpass of 1.0 nm. The total-ozone algorithm uses the four longest wavelength bands (312.5, 317.5, 331.2, and 339.8 nm), whereas the profiling algorithm uses the shorter wavelengths. The photometer operates at 343 nm with a 3.0-nm bandpass and was designed to measure the reflectivity of the surface in the instantaneous field of view (IFOV). The SBUV also makes periodic measurements of the solar flux by deploying a diffuser plate into the field of view (FOV) to reflect sunlight into the instrument.

The monochromator and the photometer are mounted so that they look in the nadir direction with coincident FOV's of 11.3 by 11.3 degrees. As the satellite moves in a Sun-synchronous retrograde orbit, the FOV traces 200-km wide paths on the ground separated by 26-degree longitude intervals. The satellite footprint moves at a speed of about 6 km/sec, and the interval between consecutive SBUV scans is 32 seconds. The order of measurements is 339.8 to 255.5 nm and the integration time is 1 second per measurement. For each monochromater measurement there is a photometer measurement.

1.3 THEORETICAL FOUNDATIONS

The UV radiance received at the satellite in the total-ozone bands consists mainly of solar radiation that has penetrated through the stratosphere and has been reflected back by the dense tropospheric air and the surface. Ozone, being concentrated in the stratosphere above the region in which most of the radiation is scattered, acts as an attenuator of this radiation. By determining the amount of attenuation in the ozone absorption band, the amount of ozone above the reflecting surface can be accurately estimated. More than 90 percent of the ozone is located above the tropopause, and all clouds, most of the aerosols, and approximately 80 percent of the atmosphere are located beneath it. This almost complete separation of the ozone from the scatterers and reflectors minimizes errors caused by vertical profile shape, clouds, aerosols, and other tropospheric variables.

Several important variables are necessary for computing the theoretical intensity, I, of the backscattered ultraviolet (BUV) light at the 13 SBUV wavelengths. The pressure, P_o, and the reflectivity, R, of the reflecting surface in the IFOV must be determined. The solar zenith angle, θ_o, is needed for calculating the optical slant path, $S(= 1 + \sec \theta_o)$, of the UV light down through the atmosphere and back to the satellite.

The total backscattered radiance, I, for π units of incident solar flux at wavelength λ can be expressed as the sum of two terms after Dave[3] as follows:

$$I(\lambda, \Theta_o, R, P_o, \Omega, \mathcal{J}) = I_o(\lambda, \Theta_o, P_o, \Omega, \mathcal{J}) + \frac{T\ (\lambda, \Theta_o, P_o, \Omega, \mathcal{J})}{1 - RS^b(\lambda, P_o, \Omega, \mathcal{J})} \qquad (1)$$

where T is the atmospheric transmission, S^b is the atmosphere to surface backscatter fraction, and Ω is the total ozone. The arguments specify the independent variables in the computation. The symbol, $\mathcal{J}$, signifies the dependence on ozone profile shape.

The first term of equation 1, I_o, is the purely atmospheric backscattered radiation intensity--the intensity at zero surface reflectivity. The second term accounts for the direct and diffuse radiation reflected by the surface. The ratio, I/F (sometimes called the geometric albedo), where F is the incident solar flux, is used to determine total-ozone and ozone profiles.

Because they are more sensitive to ozone absorption, the shorter wavelengths are used to determine the vertical ozone profile. The intensity of the BUV light at the satellite is affected by the ozone distribution and the distribution of air molecules. Thus, the ozone distribution is most easily determined in terms of the distribution of air molecules (i.e., as a function of pressure, p). The BUV intensity, I_λ, at wavelength λ can be expressed by:

$$I_\lambda = \beta_\lambda \cdot P(\cos \Theta_o) \frac{F_\lambda}{4\pi} \int_o^{P_o} e^{-S(\alpha_\lambda x + \beta_\lambda p)}\, dp + I_{MS_\lambda} \qquad (2)$$

where

β_λ = Rayleigh scattering coefficient at wavelength λ

$P(\cos \theta_o)$ = Rayleigh scattering phase function for solar zenith angle θ_o. Using a depolarization factor of 0.035, this can be written as $0.7629\ (1 + 0.932 \cos^2 \theta_o)$

F_λ = incident solar flux at wavelength λ

p_o = pressure at the bottom of the atmosphere

s = optical slant path for a plane parallel atmosphere ($= 1 + \sec \theta_o$)

α_λ = ozone absorption coefficient at wavelength λ

x = ozone overburden at pressure p

The term, $I_{MS\lambda}$, represents the multiple scattered and reflected intensity. The integral term gives the single scattered intensity. If a Q-value is defined as :

$$Q_\lambda = \frac{4\pi}{\beta_\lambda \cdot P(\cos \theta_o)} \left(\frac{I_\lambda}{F_\lambda}\right) \qquad (3)$$

then by using a similar definition for Q_{MS_λ}, equation 2 becomes:

$$Q_\lambda - Q_{MS_\lambda} = \int_o^{p_o} e^{-s(\alpha_\lambda x + \beta_\lambda p)}\, dp \qquad (4)$$

The right-hand side of this equation is referred to as the single scattered Q-value, and the left-hand side as the measured Q-value corrected for multiple scattered and reflected radiation. The inversion of equation 4, using the measured Q-values for each profile wavelength, yields the ozone profile.

2. THE ALGORITHM

The SBUV algorithm consists of two parts, a total-ozone algorithm and an ozone-profile algorithm. The data are input to the program from an RUT-S tape (raw units tape). In addition to SBUV data, the RUT-S has had terrain pressures, temperature/humidity infrared radiometer (THIR) cloud data, and snow/ice thicknesses merged onto it. The THIR is an instrument that is on board Nimbus 7.

2.1 TOTAL-OZONE ALGORITHM

The algorithm for deriving total ozone from backscattered radiances is fundamentally very simple. Given the solar zenith angle, θ_o, the surface reflectivity, R, and the surface pressure, P_o, the columnar amount of total-ozone, Ω, is obtained by a lookup and interpolation procedure, using a table of precomputed radiances. The following paragraphs outline the various steps of the algorithm.

2.1.1 Computation of Theoretical Radiances

The radiance tables were created by using a set of 21 climatological ozone vertical profiles.[4] These profiles were determined for three latitude bands using balloon ozonesondes. There are three profiles for low latitudes (Ω = 0.2 to 0.3 atm-cm in 0.05-atm-cm steps), eight for midlatitudes (0.2 to 0.55 atm-cm), and ten for high latitudes (0.2 to 0.65 atm-cm).

The precomputed radiance tables (called standard tables) were calculated by using the auxiliary equation solution to the radiative transfer equation.[3] The ozone absorption coefficients are based on the measurements of Inn and Tanaka,[5] using Vigroux's[6] temperature coefficients. The computation of the band-average coefficients is described by Klenk.[7] These absorption coefficients are listed in Table 1. The reflecting surface is assumed to be Lambertian. For each of the 21 standard profiles, radiances are computed for reflecting surface pressures of 1.0 and 0.4 atm. The tables have an upper limit on the solar zenith angle of 85.7 degrees.

2.1.2 Computation of Normalized Radiances (I/F)

The algorithm calculates a nominal value of the solar flux, F, using the prelaunch irradiance calibration constants and measurements made soon after launch, as follows:

$$F_\lambda = K_\lambda \cdot C_\lambda (d_o) \cdot F_1 (\alpha,\beta)\ R^2(d_o) \tag{5}$$

where

F_λ = solar flux at wavelength λ normalized to 1 AU

K_λ = irradiance calibration constant at λ

$C_\lambda(d_o)$ = measured counts at wavelength λ on day d_o, the first measurement of the solar flux after launch

$F_1(\alpha,\beta)$ = angular response function of the diffuser plate

$R^2\ (d_o)$ = Sun/Earth distance on day d_o in AU

$= 1-0.0167 \cos (2\pi(d_o-4)/365.25)$

A nominal value of the backscattered intensity is also calculated:

$$I_\lambda = K_\lambda \cdot C'\ (d) \tag{6}$$

Table 1
External Inputs

Wavelength (nm)	Effective Ozone Absorption Coefficient (atm-cm^{-1})	Rayleigh Scattering Coefficient (atm^{-1})	Solar Flux (watt/cm^3/AU)	Prelaunch Radiance Calibration constant (watt/cm^3/ster/count) (gain range 2)
255.652	297.3	2.4526	76.09	5.102×10^{-5}
273.608	162.6	1.8198	186.6	5.506×10^{-5}
283.099	76.50	1.5688	315.4	5.978×10^{-5}
287.702	45.32	1.4628	323.2	6.157×10^{-5}
292.289	26.32	1.3663	528.7	6.274×10^{-5}
297.586	13.18	1.2650	508.9	6.352×10^{-5}
301.972	7.300	1.1881	439.9	6.366×10^{-5}
305.872	4.455	1.1245	567.1	6.347×10^{-5}
312.565	1.750	1.0250	670.8	6.268×10^{-5}
317.561	0.9209	0.9580	773.2	6.188×10^{-5}
331.261	0.1675	0.8005	987.7	5.203×10^{-5}
339.892	0.0406	0.7183	1043.6	4.463×10^{-5}
343.3 (photometer)	0.0191	0.688	972.0	1.853×10^{-3}

where

$C'_\lambda(d)$ = measured BUV counts at wavelength λ on day d

k_λ = prelaunch radiance calibration constant

A corrected value of I/F is obtained from the nominal values of I and F by multiplying by a time-varying correction function, F'_2, given in Appendix A.

$$\left(\frac{I}{F}\right)_{\text{corrected}} = \left(\frac{I_\lambda}{F_\lambda}\right) \cdot R^2(d) \cdot F'_2(t) \tag{7}$$

The correction function, $F'_2(t)$, accounts for any changes in the solar output with time and for any changes in the instrument throughput with time. For the calculation of the albedos (I/F), instrumental and solar-flux changes need not be known separately. Note, however, that the $F_2(t)$ functions were obtained by assuming that the optical characteristics of the diffuse solar reflector did not change since the prelaunch calibrations. Stability of this reflector is important because it is the only optical component that is used for solar-flux measurements but not for radiance measurements. On the basis of studies of equatorial radiances, it is believed that the diffuser plate reflectance was stable within 2 percent at 339.8 nm during the first year of satellite operation.

It is convenient to convert the albedos into an attenuation number, called an N-value, defined as:

$$N_\lambda = -100 \log_{10}\left(\frac{I_\lambda}{F_\lambda}\right) \tag{8}$$

2.1.3 Calculation of Reflectivity

For wavelengths in which no ozone absorption occurs, the measured radiance, I_M, can be used to infer the reflectivity of the IFOV. Removing the ozone dependence from equation 1 and solving for the reflectivity, R,

$$R = \frac{I_M - I_o(\lambda, \Theta_o, P_o)}{T(\lambda, \Theta_o, P_o) + S^b(\lambda, P_o) \cdot \left[I_M - I_o(\lambda, \Theta_o, P_o)\right]} \tag{9}$$

where I_o, T, and S^b are computed from the standard tables. The two longest SBUV wavelengths--the 343-nm photometer and the 339.8-nm monochrometer channel--are slightly inside the ozone absorption band. Fortunately, at these wavelengths, the amount of ozone needs to be known only approximately (±0.05 atm-cm) for the error in the reflectivity attributable to ozone contamination to be less than 1 percent.

The 343-nm filter photometer has experienced continued degradation during the first year of data. It is anticipated that it will eventually not be sensitive enough to accurately determine the reflectivity. It has therefore been decided to exclusively use the 339.8-nm monochromator channel for determining reflectivity to avoid a discontinuity in the data when the photometer becomes unusable. However, the photometer is still used to account for scene changes between different wavelength steps of the monochromator, which, in extreme cases, could be as large as 5 percent per step.

2.1.4 Calculation of Total Ozone

A-pair and B-pair N-values used in the total-ozone algorithm are defined as:

$$N_A = N_{312.5} - N_{331.2} \tag{10a}$$

$$N_B = N_{317.5} - N_{339.8} \tag{10b}$$

The algorithm calculates the total ozone by a simple linear interpolation between adjacent N-values in the standard tables. This is done for each of the two pressure levels of the tables--1.0 and 0.4 atm--to be combined later according to the IFOV pressure. (See next page.)

An important step is the selection of the proper set of climatological standard tables from the three sets available. When the solar zenith angle is less than 78.5 degrees ($S < 6.0$), this decision is made entirely on the basis of the latitude of the IFOV as follows:

Latitude (degrees)	Use
0 to ±20	Low-latitude tables
±20 to ±30	Mix low- and mid-latitude tables
±30 to ±60	Mid-latitude tables
±60 to ±70	Mix mid- and high-latitude tables
±70 to ±90	High-latitude tables

Abrupt discontinuities in total ozone are avoided by using a linear mixture by latitude of two of the tables in the latitude mixing regions.

A different table selection scheme is used when the solar zenith angle is 78.5 degrees or greater ($S \geq 6.0$) because of the increased sensitivity of total ozone to the profile shape. This selection is made between the mid- and high-latitude tables on the basis of the measured A-pair N-value, N^A_{meas}. Theoretical A-pair N-values are interpolated from the tables, using the B-pair mid- and high-latitude ozone values $\left(\Omega^B_{mid} \text{ and } \Omega^B_{high}\right)$, giving N^A_{mid} and N^A_{high}.

The weight used in mixing the mid- and high-latitude tables is then obtained as follows:

$$\text{WEIGHT} = \frac{N^A_{meas} - N^A_{mid}}{N^A_{high} - N^A_{mid}} \qquad (11)$$

This weight is then used to combine the two ozone values as follows:

$$\Omega^B = \Omega^B_{high} \cdot \text{WEIGHT} + \Omega^B_{mid} \cdot (1 - \text{WEIGHT}) \qquad (12)$$

A "table index"(= WEIGHT + 2.0) is calculated to indicate how the mid- and high-latitude tables were mixed. To avoid a discontinuity, total-ozone values calculated from the low and the high zenith angle (ZA) methods are combined linearly by slant path between S = 6.0 and S = 8.0. Thus, not until ZA = 81.8 degrees (S = 8.0) is the new method in full force. Note that, in the high ZA method, A-pair ozone is not calculated.

2.1.5 Calculation of IFOV Pressure

The average pressure of the reflecting surface in the IFOV must be determined in order to properly combine the 1.0- and 0.4-atm ozone values. Two methods are used in the algorithm to find this pressure: (1) using the reflectivity and (2) using data from the THIR instrument.

2.1.5.1 Method 1--In the first method, the terrain pressure is combined with the cloud-top pressure according to the reflectivity and the presence or absence of snow. A latitude-dependent climatological average cloud-top pressure obtained from THIR studies is calculated according to:

$$P_{cloud} = 0.3 + 0.15 \left[1 - \cos\,(2 \cdot \text{lat})\right] \text{ atm} \qquad (13)$$

The average IFOV pressure, P_o, is obtained as follows:

$$P_o = f \cdot P_{cloud} + (1 - f) \cdot P_{terrain} \tag{14}$$

where the estimated fractional cloudiness, f, is obtained by using the measured reflectivity, R, and snow/ice information as follows:

	No Snow	With Snow (>0.5 inches thick)
$R \leq 0.2$	$f = 0$	$f = 0$
$R \leq 0.6$	$f = 1$	$f = 0.5$
$0.2 < R < 0.6$	$f = \frac{R - 0.2}{0.4}$	$f = \frac{R - 0.2}{0.8}$

2.1.5.2 Method 2--The second method uses THIR cloud data when available. THIR 11.5-μm radiances are used to determine the cloud-top pressure, P_{cloud}, and the fractional cloudiness, f, in the SBUV IFOV. These quantities are contained on the RUT-S tape. The equation for the THIR-derived pressure is identical to equation 14.

Because the ozone retrieval is very sensitive to the IFOV pressure at low reflectivities, limits are set on the use of THIR. For $R \leq 0.2$, terrain pressure is used regardless of THIR. To prevent unreasonably low THIR pressures, a latitude-dependent minimum allowable cloud-top pressure is defined, as follows:

$$P_{cloud}^{min} = \left[0.1 + 0.15 \quad 1 - \cos\,(2 \cdot lat)\right] \text{ atm} \tag{15}$$

This is used to compute a minimum acceptable THIR pressure given by:

$$P_{THIR}^{min} = f \cdot P_{cloud}^{min} + (1 - f) \cdot P_{terrain} \tag{16}$$

The fractional cloudiness in equation 16 is determined from the reflectivity and snow/ice thickness as in method 1. The actual THIR

IFOV pressure is reported on the ozone tape, but, if it is less than P_{THIR}^{min}, the total-ozone calculations are made, using P_{THIR}^{min}.

When IFOV pressures are determined, both a reflectivity-derived and a THIR-derived ozone are calculated for each pair (or for B-pair only at ZA ≥ 78.5 degrees) by a linear interpolation of the ozone values derived by using the 1.0- and the 0.4-atm tables. The ozone values calculated represent the total ozone down to the terrain height. In the presence of clouds, the reported ozone implicity includes a climatologically determined amount of ozone below the cloud.

2.1.6 Calculation of Best Ozone

After adjusting for the IFOV pressure, the A-pair and B-pair ozone values are combined to get a single "best" ozone estimate. The weighting of the A- and B-pair ozone is done on the basis of the slant path, S. At small values (S ≤ 2.5), the A-pair ozone is preferable because algorithmic errors are usually larger for the B-pair ozone. At large values (S ≥ 5.0), the B-pair ozone is preferable because the A-pair becomes more sensitive to the shape of the ozone profile. Because, at intermediate values of the slant path, the A- and B-pair sensitivities to the ozone profile and to algorithmic errors are comparable, a weighted mean is taken as the best ozone. Thus, best ozone, $_{Best}$, is computed as:

$$\Omega_{Best} = \Omega_A \qquad (S \le 2.5) \qquad (17a)$$

$$\Omega_{Best} = \frac{\Omega_A\,(5.0 - S)}{2.5} + \frac{\Omega_B\,(S - 2.5)}{2.5} \qquad (2.5 < S < 5.0) \qquad (17b)$$

$$\Omega_{Best} = \Omega_B \qquad (S \ge 5.0) \qquad (17c)$$

2.1.7 Validity Checks

The algorithm contains several validity checks for maintaining data quality. In processing before the ozone determination, several checks are made on the solar zenith angle, satellite attitude, and instrument status to ensure the quality of the radiances and other geophysical input. This section describes the quality checks performed on the derived reflectivity and ozone to identify bad scans caused by either bad input that passed preprocessing checks or limitations of the ozone algorithm. A flow chart of the quality checks is shown in Figure 1.

The computed total ozone for each pair must be within the dynamic range of the radiance tables. For low, mid, and high latitudes, the ranges are 0.18 to 0.35, 0.18 to 0.60, and 0.18 to 0.65 atm-cm, respectively. If A- or B-pair ozone exceeds the range, it is set to -999, best ozone is set to -999, and quality flag = 9 is assigned.

Next, a check is made on the best reflectivity. The reflectivity must be no less than -0.05 and no greater than +1.05. If this range is exceeded, the best ozone is set to -999, and quality flag = 8 is assigned.

A second check is made on the reflectivity. Even though the 343-nm photometer reflectivity is not used in the total-ozone computation, it is used as a check on the 339.8-nm monochromator reflectivity. If these two differ by more than 0.15, the best ozone is set to -999, and quality flag = 7 is assigned. Significant differences in the two reflectivities could result from instrument calibration errors or significant departure of the real atmosphere and surface from the algorithmic model.

If the data pass flags 9, 8, and 7, the slant-path length ($1 + \sec \theta_o$) is checked. Two additional checks are made on low solar zenith angle data ($S < 6.0$), and three are made on high solar zenith angle data ($S \geq 6.0$).

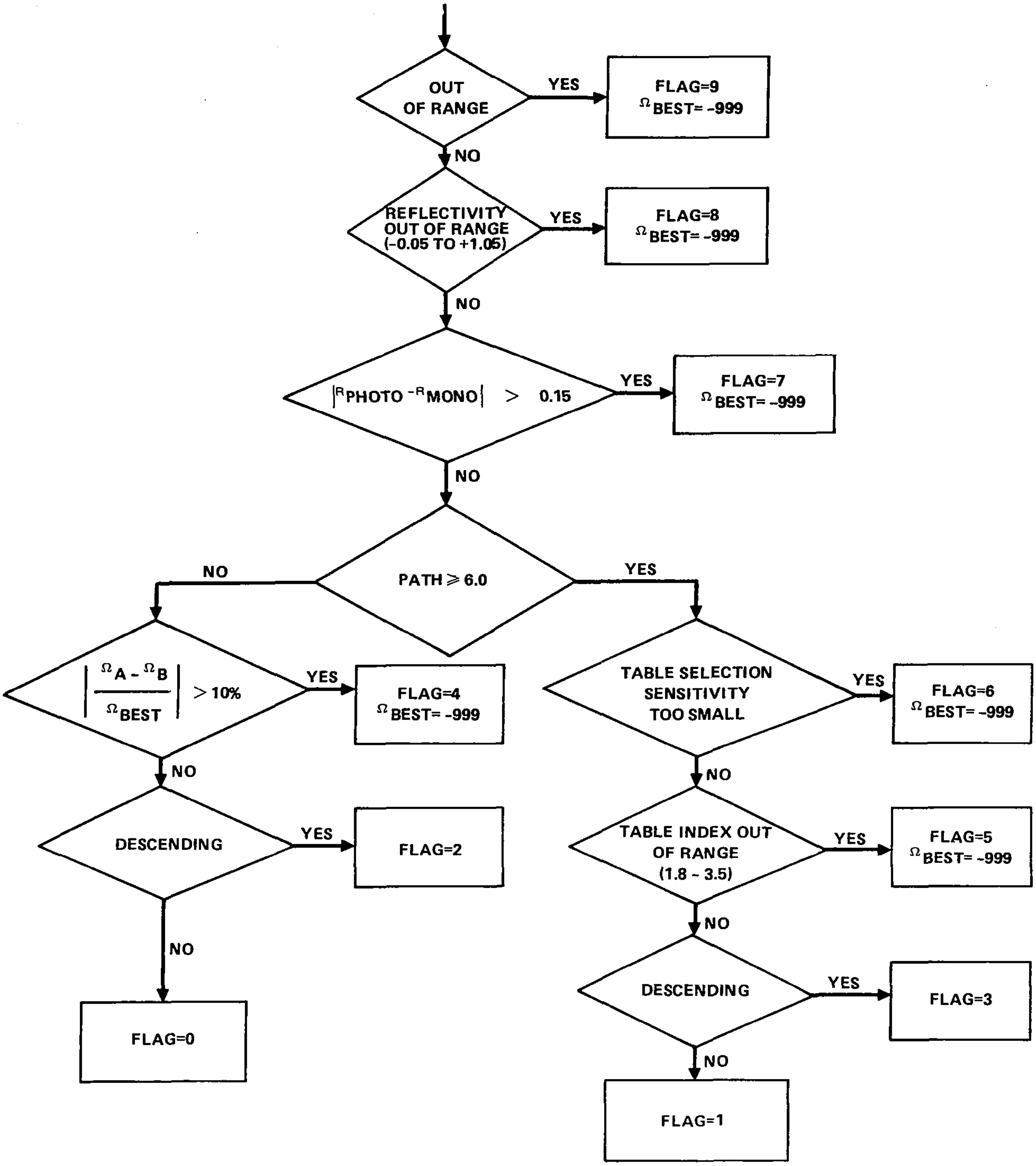

Figure 1. Quality Flags

For low solar zenith angle data, the difference between the A-pair and B-pair ozone is checked. If the difference exceeds 10 percent of the best ozone, quality flag = 4 is assigned and the best ozone is set to -999.

Low zenith angle data that pass flag 4 can be considered to be good data. A final check is made to determine if the scan occurred during the ascending or the descending part of the orbit. Although, for the most part, the satellite is over the dark side of the Earth during the descending part of the orbit, it is possible to retrieve ozone from both the ascending and descending parts of the orbit during summer when the polar region is in sunlight. Descending scans are assigned quality flag = 2, and a normal best ozone is reported. If the scan is an ascending scan, quality flag = 0 is assigned.

Ascending scans are preferable to descending scans at the same latitude because the solar zenith angle is smaller. Descending data are taken at a local time several hours different from local noon time, when most of the SBUV data are taken. Also, Dobson stations usually make measurements around local noon. Thus, the use of descending data should be avoided when diurnal variations are important, as in zonal means or Dobson comparisons.

For high solar zenith angle data, the sensitivity of the table selection scheme is calculated. If the sensitivity is low, quality flag = 6 is assigned, and the best ozone is set to -999. Low sensitivity means that the table selection scheme is only weakly sensitive to differences between the mid- and high-latitude profiles.

The table index is also checked for high solar zenith angle data. The table index must be no less than 1.8 and no greater than 3.5. Studies of the table selection scheme have shown that these limits are rarely exceeded. This prevents the effective selected profiles from varying too much from either mid- or high-latitude profiles.

If the limits are exceeded, quality flag = 5 is assigned, and the best ozone is set to -999.

For the same reasons as for the low solar zenith angle, the high zenith angle data that have passed all other checks is checked last for being in the ascending or descending part of the orbit. Descending scans are assigned quality flag = 3, ascending scans are assigned quality flag = 1, and a best ozone is reported for both.

2.2 PROFILE ALGORITHM

Determination of the vertical ozone profile requires the inversion of equation 4 by using an optimum statistical technique described by Rodgers.[8] The application of this technique to the SBUV data is described by Schneider _et_ _al_.[9] and will only be outlined here. The wavelengths from 273.5 to 305.8 nm are used for profiling. In addition, at solar zenith angles greater than 75.50 degrees, the 312.5-nm radiance is also used. The optimum method yields the ozone layer amounts (the solution profile) and their standard deviations (solution profile covariance matrix) in 12 atmospheric layers defined by pressure. Mixing ratios for 16 meteorological levels (0.3, 0.4, 0.5, 0.7, 1.0, 1.5, 2.0, 3.0, 4.0, 5.0, 7.0, 10, 15, 20, 30, and 40 mbars) are also calculated from the layer amounts. The various steps in the profile algorithm are outlined below.

2.2.1 Inversion to Obtain Profile

To linearize the integral equation, the ozone profile is represented by 12 unknowns that represent the ozone amounts in 12 layers. The pressure at the bottom of each layer (0.24, 0.49, 0.98, 1.95, 3.9, 7.8, 15.6, 31, 62, 125, 250, and 1000 matm-cm) is the same as that of the Umkehr layers but it is reversed. The layer thicknesses are thin enough to permit the full resolution of profile data that the indirect method is capable of.

The integral equation is expanded by a Taylor series in terms of the natural logarithm of the single scattered component of the measured Q_λ:

$$\ln (Q_\lambda - Q_{MS}) = \ln Q'_{SS} + \sum_{k=1}^{12} \left(\frac{\partial \ln Q_{SS}}{\partial \ln X_k} \right)_{X'} \left[\ln X_k - \ln X'_k \right] \qquad (18)$$

where SS implies the single scattering term, MS implies the multiple scattering term, X_k is the ozone amount in the kth layer, and the prime denotes the result of the previous iteration.

A priori information in the form of a predicted climatological profile and an associated covariance matrix (paragraph 2.2.3) are provided for the inversion. The standard deviations and correlations between the Q-values (the measurement covariance matrix) are also input. The solution is obtained by minimizing the weighted sum of the squares of the differences between the logarithms of the observed and calculated Q-values and the difference between observed and calculated total-ozone values under the constraint that the solution profile differs minimally from the *a priori* profile. The constraints are imposed in a statistically optimum manner by including the full covariance matrix of the radiance errors and errors in estimating the *a priori* profile. Two to three iterations normally suffice. In addition to the solution profile (the 12 layer amounts), a solution profile error covariance matrix (the standard deviations) is also obtained.

2.2.2 Calculation of Multiple-Scattering Component

Multiple scattering, which occurs in the troposphere, is important only at wavelengths longer than 290 nm. The multiple-scattering terms for the longer wavelengths are computed before the solution process and are kept fixed. Multiple scattering is weakly dependent on the profile shape (see Taylor et al.[10]) but are strongly dependent on the total ozone, the solar zenith angle, the surface pressure, and the surface reflectivity. Although the reflectivity is obtained by using the 339.8-nm band of the monochromator, the photometer is used to account for scene changes between the 339.8-nm measurement and those at the profile wavelengths.

Multiple-scattering Q-values are tabulated for three latitude bands in terms of total ozone and optical path length. Low- and mid-latitude values are used from +45 to -45 degrees latitude. Mid- and high-latitude values are used from ±45 degrees to the poles. Interpolation between latitude bands is done linearly by comparing the observed Q with the two calculated Q's. If the Q is outside the range of the calculated Q's, the latitude band whose Q is nearest the observed Q is used. The amount of interpolation in latitude between the multiple-scattered Q-values is specified for each wavelength by the multiple-scattering mixing fraction, in which values of 1.0, 2.0, and 3.0 indicate the low-, mid-, and high-latitude bands, respectively.

As part of the interpolation process for determining the multiple-scattering Q-value, the sensitivity of the multiple-scattering Q-value to total ozone is calculated for each of the longer wavelengths. The sensitivity is the partial derivative of the multiple-scattering Q-value with respect to total ozone and is used to calculate the variances and covariances associated with the multiple-scattering component of Q for the measurement covariance matrix.

2.2.3 A Priori Profile and Covariance Matrix

The *a priori* profile and its covariance matrix represent the quantitative knowledge of the amount of ozone in each layer of the atmosphere as a function of latitude and time. The amount of ozone in each kth layer is given by:

$$X_k = A_k + \left[1-\cos\,(2\cdot\text{lat})\right] \left[B_k + C_k \cdot \cos\left(\frac{2\pi}{365}(d-\phi_k)\right)\right] \qquad (19)$$

where

A_k = ozone in layer k at the Equator

B_k = change in yearly average ozone in layer k in going from the Equator to 45 degrees latitude

C_k = amplitude of the annual wave in the kth layer at 45 degrees latitude

ϕ_k = day of the peak of the annual variation in the Northern Hemisphere ($\phi_k' = \phi_k$ + 182.5 days in the Southern Hemisphere)

lat = latitude

d = day of the year

Table 2 lists the coefficients for each layer, and Table 3 gives the a priori profile error covariance matrix assumed by the retrieval algorithm. This matrix gives the covariances of the fractional difference between the measured layer ozone amounts from those predicted by equation 19. This covariance matrix is used for all measurements. Nimbus 4 BUV data from 1971 were employed to obtain the coefficients and covariance matrix elements for the layers above 16 matm. For the lower layers, the ozonesonde data set compiled by the Atmospheric Environment Service, Canada, was used.

Table 2
A Priori Profile Coefficients

Layer*		Coefficients			
No. (k)	Pressure (matm)	A_k (DU)**	B_k (DU)	C_k (DU)	ϕ_k (day)
1	0 → 0.24	0.110	-0.010	0.004	0
2	0.24 → 0.49	0.250	0.010	0.040	-10
3	0.49 → 0.98	0.850	0.130	0.250	-11
4	0.98 → 1.95	3.00	0.600	1.00	-9
5	1.95 → 3.9	11.5	-0.400	0.700	4
6	3.9 → 7.8	33.0	-7.400	1.90	164
7	7.8 → 15.6	62.0	-19.0	2.40	154
8	15.6 → 31	75.0	-6.00	0.00	-
9	31 → 62	44.0	38.0	13.0	59
10	62 → 125	5.00	49.0	16.0	62
11	125 → 250	3.00	25.0	12.0	91
12	250 → 1000	15.0	10.0	8.0	182

*Although the pressure range of the layers defined here are identical to those used for Umkehr retrievals, the numbering scheme is the reverse of that for Umkehr, for which the numbers increase with height.

**DU = Dobson units.

Table 3
A Priori Profile Error Covariance Matrix*

Layer Number	1	2	3	4	5	6	7	8	9	10	11	12
1	22.50	12.60	4.29	0	0	0	0	0	0	0	0	0
2		14.40	9.24	2.28	0	0	0	0	0	0	0	0
3			12.10	7.70	0.97	0	0	0	0	0	0	0
4				10.00	4.16	-0.72	0	0	0	0	0	0
5					6.40	2.18	-1.04	0	0	0	0	0
6						6.40	4.00	0	0	0	0	0
7							10.00	5.76	0	0	0	0
8		MATRIX SYMMETRICAL ABOUT DIAGONAL						14.40	10.08	-0.36	0	0
9									22.50	17.55	7.35	0
10										90.00	89.67	6.30
11											240.1	53.17
12												122.5

*All elements must be multiplied by 10^{-3}. Layer numbers are identical to those in Table 2.

2.2.4 Measurement Covariance Matrix

The measurement covariance matrix specifies uncertainties in the measured and calculated Q-values and any correlations that might exist between these errors. Diagonal elements of the covariance matrix contain a sum of the square of three errors: a 0.5-percent instrument error, error in radiances due to an assumed 1-percent error in ozone absorption coefficients, and error in multiple scattering corrections due to a 2-percent error in total ozone (applies only to wavelengths longer than 292.3 nm). These errors are computed for each SBUV scan because they vary with solar zenith angle and surface reflectivity. The combined rms errors vary from ~0.7 percent for the shortest wavelengths to as much as 10 percent for the longest wavelengths for scenes containing clouds. Off-diagonal terms of the covariance matrix are caused by total-ozone errors that cause correlated errors in multiply-scattered wavelengths. (For more details, see Section 3 of Schneider *et al.* [8])

2.2.5 Validity Checks

Several checks are made to identify scans with missing or grossly abnormal values. If the scan fails any one of these checks, a profile error code is assigned.

If any profile wavelength measurements are missing, a profile error code of 1 is assigned. If a best-ozone value has not been computed in the total-ozone algorithm, then a profile error code of 2 is assigned. If the monochromator reflectivity for any wavelength is outside the range -0.05 to +1.05, or if the reflectivity changes by more than 0.05 from wavelength to wavelength, then a profile error code of 3 is assigned.

The algorithm uses the 274- and 283-nm Q-values to calculate values for C, the cumulative ozone at 1 mbar, and σ, the ratio of the atmospheric scale height to the ozone scale height, assuming that the cumulative ozone, X, is a function of the pressure, p:

$$X = C\, p^{1/\sigma} \tag{20}$$

If σ is outside the range from 0.3 to 0.8, a profile error code of 4 is assigned. If C is greater than 3.0 matm-cm or less than 0.5 matm-cm, a profile error code of 5 is assigned.

If the observed Q-value differs by more than 60 percent from the Q-value calculated from the a priori profile and the tabulated multiple-scattering Q's, a profile error code of 6 is assigned.

For error codes 1 through 6, the profile solution is terminated as soon as the error code is assigned. The function of error codes 4, 5, and 6 is to prevent grossly abnormal Q-values from being used as input to the algorithm. These may result from momentary lapses in the instrument performance or the data transmission and storage process. Profile error code 7 is not currently used.

If the scan passes checks 1 through 6, the ozone profile is computed, and two additional checks are made. If the atmospheric pressure at which the cumulative ozone is one half of the total ozone is not between 10 and 100 mbar, the profile is considered suspicious, and a profile error code of 8 is assigned. If the ozone mixing ratio between 0.3 and 40 mbars exceeds 23 μgm/gm, the profile is also considered suspicious, and a profile error code of 9 is assigned. If the profile passes these checks, it is considered a good profile, and a profile code of 0 is assigned.

3. TAPE FORMATS

The SBUVALL program creates an output tape called the OZONE-S tape. This tape can be described in terms of its physical structures and/or in terms of its logical structure.

3.1 PHYSICAL STRUCTURE OF OZONE-S TAPE

The OZONE-S tape is a multiple-file binary tape written in fixed-block (FB) format on an IBM 360 machine. It contains a header file, followed by files for each orbit of data and, finally, a trailer file.

The first file is a special file called the standard header, which is written in a format common to all archivable tapes produced by the Nimbus Operational System (NOPS). This file contains two identical blocks of 630 characters written in EBCDIC. Each block consists of five 126-character lines.

Lines 1 and 2 are written according to a standardized format called the NOPS Standard Header Record. The standard header records contain the following information:

- Nimbus-7 NOPS tape product format specification number consisting of 30 characters. For all OZONE-S tapes, the character string is ${}_b$NIMBUS-7${}_b$NOPS${}_b$SPEC${}_b$NO${}_b$T634041. The subscript "b" indicates a blank.

- Tape sequence number consisting of a two-character code identifying the tape (for OZONE-S this is FE) a 5-character sequence number unique to each tape, a hyphen, and a one-digit number specifying the copy number. An example for an OZONE-S tape is FE83231-2.

- Subsystem identification code consisting of 4-characters preceded and followed by blanks. For OZONE-S, this is $_{b}\text{SBUV}_{b}$.

- Generation and destination facilities consisting of four characters each are given. An example is $\text{SACC}_{b}\text{TO}_{b}\text{IPD}_{b}$. In this example SACC is the computer facility that generated the OZONE-S tape and IPD in the destination of the tape.

- The beginning and ending dates of data coverage are given as $_{b}\text{START}_{b}\text{19YY}_{b}\text{DDD}_{b}\text{HHMMSS}_{b}\text{TO}_{b}\text{19YY}_{b}\text{DDD}_{b}\text{HHMMSS}_{b}$ where YY is the year, DDD is the Julian day of the year, HHMMSS are the hour, minute, and second of the day. For the OZONE-S tape, the ending date is not the true ending date of the data on the tape but a fill date (i.e., $1999_{b}365_{b}002400$). In order to avoid unnecessary processing complications, the true ending date does not appear in the header record.

- The tape generation date is given in a similiar format as above: $\text{GEN}_{b}\text{19YY}_{b}\text{DDD}_{b}\text{HHMMSS}_{b}$.

The following character string is an example of an OZONE-S header record:

```
NIMBUS-7 NOPS SPEC NO T634041 SQ NO FE83231-2 SBUV SACC TO IPD
START 1978 328 090427 TO 1999 365 002400 GEN 1981 106 115029
```

Lines 3, 4, and 5 are used by the subsystem analyst for further identification of the data tape. Line 3 of the header file is usually left blank. Lines 4 and 5 contain information about the processing software such as program name, version number, and version date.

The remaining files on the tape each contain a variable number of blocks, each of which is 16,560 bytes long. The first word of each block contains a 32-bit block identifier (Figure 2).

BITS:	1-12	13-16	17	18	19-24	25-32
	BLOCK NUMBER ON TAPE	Spare	1 For Last Block On File	1 For Last File	Record ID's: (in decimal) 03-First block on data files 18-Intermediate blocks on data files 53-Last block on data files 58-All blocks trailer file	Spare

Figure 2. Block Identifier

3.2 LOGICAL STRUCTURE OF TAPE

The IPD header file is followed by the data files, one for each orbit of data on the tape. For most users of the tapes, it will be more convenient to treat the data files as a collection of logical records, each 828 bytes long. (Note that 20 of these records are blocked together before writing on the tape.)

The first record of each file contains processing information about the data that follows. Its format is described in Table 4. Each of the following records contain total-ozone and profile information from a single 32-second scan of the SBUV instrument. The format for these data records is given in Table 5. Typically, the SBUV takes 90 to 100 scans during the daylight half of each orbit; therefore, under normal operating conditions, one file on the tape should contain as many data records.

The last record of useful information on each file is described in Table 6. This record follows the last data record of the file and contains a processing summary of the preceding orbit of data. Following this "last" record will be dummy records to fill the last block. These dummy records keep all blocks the same length and should be ignored.

The record type can be identified by word 2 of each record. It contains the logical sequence number of records within the file. It begins at 1 for the first record of the file and is incremented by 1 for each successive record. For the last record, which contains the file processing summary (and dummy records following), the negative of the logical sequence number is written.

The last file on the tape is called the trailer file. It contains 20 identical copies of a trailer record (to fill one block), which is described in Table 7. It contains a processing summary of the entire tape, similar to that of the last record of each data file. The trailer-file records can be identified by their logical sequence number of -1.

Table 4
Format of First Record on Data Files*

4-Byte Words	Description
1	Block identifier (Figure 2)
2	Logical sequence number (1)
3	Orbit number
4-7	Date of job run (MON DEC 10, 1978)
8	Day of first good scan
9	GMT of first good scan (seconds)
10	Year of first good scan
11	Subsatellite latitude for first scan (degrees)
12	Subsatellite longitude for first scan (degrees)
13	GMT of right ascending node of orbit
14-17	Processing parameters
18-30	13 solar irradiance values (1 for each wavelength)
31-67	37 radiance conversion factors
68-80	13 instrument wavelengths
81-93	Ozone absorption coefficient for instrument wavelengths
94-106	Rayleigh scattering coefficients (atm^{-1})
107-126	20 processing options
127-207	Spare (-77)

(Continued)

*Word 1 contains hexadecimal data, words 4 to 7 contain EBCDIC data, and the remaining words contain data in IBM floating-point format (R*4).

Table 4 (Continued)

Detailed Description of First Record on Data Files	
Word	Comments
11	Latitudes range from -90 to +90 degrees, southern latitudes being negative.
12	Longitudes range from -180 to +180 degrees, western longitudes being negative.
14-17	The following processing options are currently implemented: Maximum solar zenith angle (word 14) Minimum latitude (word 15) Maximum latitude (word 16)
18-30	The solar irradiance for the current day is given in units of watts/cm^3/AU in the order words: 18:255.5, an ..., 29:339.8 nm, 30: photometer (343 nm).
31-67	The counts to radiance conversion factors are in the units of watt/cm^3/steradian/count and are given for each monochromator wavelength for each of the three gain ranges in the order words: 31-33:255.5, ..., 64-66:339.8 nm, word 67 has the value for the photometer.
68-80	Instrument wavelengths are given in nm in the same order as the solar flux.

(Continued)

Table 4 (Continued)

Detailed Description of First Record on Data Files	
Word	**Comments**
81-93	The ozone absorption coefficients for each of the foregoing wavelengths are in units of $(\text{atm-cm})^{-1}$ with base e.
107-126	There are 20 possible processing options, only, 6 of which are currently implemented (0 - disabled, 1 - enabled): Word 107--THIR processing WORD 108--Check remaining central processing unit and input/ouput time Word 112--Profile processing Word 113--Do not use 301.9-nm channel in profile processing Word 114--Do not use 255.5-nm channel in profile processing Word 115--Do not use 312.5-nm channel in profile processing

Table 5

Data Record Format for OZONE-S Tape

4-Byte Words	Description
1	Block identifier (ZXO 800); X = block number
2	Logical sequence number (N+1); N = number of data records
3	Orbit number
4	Julian day of year at the start of scan
5	GMT (seconds)
6	Subsatellite latitude at the beginning of scan (degrees)
7	Subsatellite longitude at the beginning of scan (degrees)
	Total-Ozone Output
8	View latitude--Average for total ozone (degrees)
9	View longitude--Average for total ozone (degrees)
10	Solar ZA--Average for total ozone (degrees)
11-14	Four photometer N-values (339.8, 331.2, 317.5, 312.5 nm)
15-18	Four monochromator N-values (339.8, 331.2, 317.5, 312.5 nm)

(Continued)

Table 5 (Continued)

4-Byte Words	Description
19	Gain selection flags for each of four λ's
20	Surface category code
21	THIR best ozone (Dobson units)
22	THIR A-pair ozone minus B-pair ozone (Dobson units)
23	THIR pressure (atm)
24	THIR average reflectivity
25	THIR percent cloudiness
26	THIR error flag for total ozone
27	A-pair ozone (Dobson units)
28	A-pair sensitivity (dN/dΩ)
29	A-pair average reflectivity
30	Spare (-77)
31-34	Repeat 27 through 30 for B-pair
35	Best ozone (Dobson units)
36	A-pair ozone minus B-pair ozone (Dobson units)

(Continued)

Table 5 (Continued)

4-Byte Words	Description
37	Pressure of reflecting surface (estimated)
38	Average reflectivity
39	Spare (-77)
40	Error flag for total ozone
41	Table selection scheme index
42	Snow thickness (inches)
43	Photometer/monochromator reflectivity difference
44	Terrain pressure (atm)
45-47	Spare (-77)
	Profile Output*
48	View latitude--Average for profile (degrees)
49	View longitude--Average for profile (degrees)
50	Solar ZA--Average for profile (degrees)

(Continued)

*All words are in IBM floating-point format (R*4) except word 1, which contains hexadecimal data. All ozone values are in dobson units (DU); 1 DU = 0.001 atm-cm. Logical record size = 828 bytes; block size = 16,560 bytes (20 LRECL/BLOCK). Any word in the record may contain -77, indicating fill data.

Table 5 (Continued)

4-Byte Words	Description
51-58	Eight photometer N-values (profile wavelengths 255.5, 273.5, 283, 287.6, 292.2, 297.5, 301.9, and 305.8 nm)
59-66	Eight monochromator N-values (profile wavelengths)
67-68	Gain selection flags for each of eight λ's.
69-80	_A priori_ profile individual ozone amounts (matm-cm) in 12 pressure layers
81	Total ozone (matm-cm) for _a priori_ profile
82-91	Q-values corrected for multiple scattering and surface reflectivity (255.5 through 317.5 nm)
92-101	Initial residuals (255.5 through 317.5 nm)
102-106	Multiple-scattering and reflectivity correction to Q for five longer wavelength channels (297.5 through 317.5 nm)
107-111	Monochromator reflectivities for five longer wavelength channels (297.5 through 317.5 nm)
112-116	Sensitivity of multiple-scattering and reflectivity correction to total ozone for five longer wavelength channels (297.5 through 317.5 nm)
117-121	Multiple-scattering mixing fraction for five longer wavelength channels (297.5 through 317.5 nm)

(Continued)

Table 5 (Continued)

4-Byte Words	Description
122-131	Final residues (255.5 through 317.5 nm)
132-143	Solution profile individual ozone amounts (matm-cm) in 12 pressure layers
144-155	Standard deviations for solution profile individual ozone amounts (matm-cm) in 12 pressure layers
156	Total ozone (matm-cm) for solution profile
157	Pressure mbar at which cumulative ozone is one half of total ozone
158-159	Parameters C and sigma (σ)
160-175	Solution mixing ratio (μgm/gm) at 16 pressure levels
176	Error flag for profile
177	Solar zenith angle at start of scan (rad x 10^4)
178	Solar zenith angle at end of scan (rad x 10^4)
179-190	Standard deviations for *a priori* profile individual ozone amounts (matm-cm) in 12 pressure layers
191-200	Standard deviations for Q-values corrected for multiple scattering and reflectivity (255.5 through 317.5 nm)

(Continued)

Table 5 (Continued)

4-Byte Words	Description
201	Number of interations for profile solution
202-207	Spares (-77)

Detailed Description of Data Record

Word	Comment
11-18	N-value is computed from each measurement as: $N = -100 \log_{10} (I/F)$ where I = measured radiance and F = measured solar irradiance.
19	Gain selection flags are packed in powers of ten with the 339.8-nm gain being the most significant decimal digit.
20	Surface category code (not used by the algorithm).
21-26	Final output of total-ozone processing using the cloud information from the THIR instrument.
28,32	Sensitivity of a pair is defined as $\Delta N_p/\Delta\Omega$, where N_p is the difference in the N-value of pair wavelengths and is the total ozone.
35-40	Final output of total-ozone processing using the cloud information as provided indirectly from the measured reflectivity.

(Continued)

Table 5 (Continued)

Word	Comment
26,40	Error flags are defined as follows: 0 - Low path length, good scan 1 - High path length, good scan 2 - Low path length, data taken in descending part of orbit (sunlit polar night) 3 - High path length, descending orbit data 4 - Low path length, A-pair and B-pair total-ozone estimates differ by more than 10 percent of the best total-ozone estimate. 5 - High path length, table index is out of range (less than 1.8 or greater than 3.5). 6 - High path length, table selection scheme total ozone has low sensitivity. 7 - Photometer reflectivity and monochromator reflectivity differ by more than 0.15. 8 - Best reflectivity out of range (less than -0.05 or greater than 1.05)

(Continued)

Table 5 (Continued)

Word	Comment
	9 - A-pair or B-pair total ozone exceeds the dynamic range of the tables. The dynamic ranges are: Latitude <25° 180 to 350 DU Latitude 25° to 55° 180 to 600 DU Latitude >55° 180 to 650 DU
59-66	N-values for 8 wavelengths in the order: word 59: 255.5, ..., 66: 305.8 nm.
67-68	Packed as in word 19, 2555 being the most significant digit of word 67 and 2922 that of word 68.
69-80	The *a priori* ozone amount in each layer is obtained by evaluating a harmonic series expression that is a function of latitude and day of year. The 12 layers are in order of increasing atmospheric pressure from the top of the atmosphere. The layer for word 69 extends from 0 to 0.24 matm. The pressures at the bottom of each succeeding layer increase by a factor of 2 and are 0.49, 0.98, 1.95, 3.9, 7.8, 15.6, 31, 62, 125, 250 matm. The final layer for word 80 extends from 250 to 1000 matm.

(Continued)

Table 5 (Continued)

Word	Comment
82-131	The following comments apply to these words: Q-values for wavelengths are as defined in Sections 1 through 3; that is: $Q = \frac{4\pi\ I}{F \cdot \beta \cdot P(\theta_0)}$ where I = intensity of the back-scattered radiation β = Rayleigh scattering coefficient F = solar flux , $P(\theta_0)$ = Rayleigh scattering phase functions The residue is defined as $\frac{Q_{obs} - Q_{msr} - Q_{ss}}{Q_{obs}}$ where Q_{obs} = Q-value obtained from the observed radiance (Continued)

Table 5 (Continued)

Word	Comment
81-131 (Cont.)	Q_{msr} = Q-value that refers only to the multiple-scattered and reflected component of the total intensity (obtained from a lookup table) Q_{ss} = Q-value that refers to the single scattered component of the total intensity (calculated within the program) An initial residue is defined as the residue for which the <u>a priori</u> (initial) profile was used in obtaining Q_{cal}. For final residues, the final retrieved profiles are used. Not that, in both cases, the values of Q_{msr} remain the same. The Q-values and other related quantities are given in order from the shorter to the longest wavelengths. In words 102 through 121, values for wavelengths shorter than 297.5 nm are assumed to be zero. Because the 317.5-nm wavelength was never used in inversion, the words reserved for it are filled with -77. Words reserved for 312.5 nm contain valid data only when this wavelength is used. (See Section 2.2.) (Continued)

Table 5 (Continued)

Word	Comment
158-159	Parameters determined by assuming an ozone profile of the form: $$x(p) = C p^{1/\sigma}$$ where p = pressure in mbar, x = cummulative ozone at pressure level p, and C = ozone at 1 mbar (DU)
160-175	Values of the solution profile mass mixing ratios are given in order of increasing atmospheric pressure at the 16 pressure levels: 0.3, 0.4, 0.5, 0.7, 1.0, 1.5, 2.0, 3.0, 4.0, 5.0, 7.0, 10, 15, 20, 30, and 40 mbar.
176	Error flags are defined as: 0 - No error 1 - Missing measurements 2 - Total ozone not available 3 - Reflectivity is less than -0.05, greater than 1.05, or changes by more than 0.05 from wavelength to wavelength 4 - Sigma greater than 0.8 or less than 0.3 5 - C greater than 3.0 DU or less than 0.5 DU

(Continued)

Table 5 (Continued)

Word	Comment
	6 - Measured Q-value differs by more than 60 percent from Q-value calculated with a priori profile and multiple-scattering/reflectivity correction 7 - Unassigned error flag 8 - Pressure at which cumulative ozone is one half of the total ozone is less than 10 mbar or greater than 100 mbar 9 - solution profile mixing ratio is greater than 23 µgm/gm

Table 6
Format of Last Record on Data Files*

4-Byte Words	Description
1	Block identifier (ZX03500); X = block number
2	Negative of logical sequence number (N+2); N = number of data records
3	Orbit number
4	Day of last scan on file
5	GMT of last scan on file (seconds)
6	Subsatellite latitude at the beginning of scan (degrees)
7	Subsatellite longitude at the beginning of scan (degrees)
Total-Ozone Output	
8	View latitude--Average for total ozone on last scan (degrees)
9	View longitude--Average for total ozone on last scan (degrees)
10	Number of tape read errors
	(Continued)

*All words are in IBM floating-point format except for word 1, which contains hexadecimal data.

Table 6 (Continued)

4-Byte Words	Description
11	Number of scans read
12	Number of scans written
13-27	Total-ozone processing counters
28-37	Profile processing counters
38-207	Spare

Detailed Description of Last Record on Data Files

Word	Comment
13-27	The following counters have been defined for total-ozone processing: Total number of scans written on the tape unprocessed (word 13): - For zenith angle too large (14) - Bad counts (16) Total number of scans written with negative best ozone (word 17): - For ozone too low/high (18) - For monochromator out of range (19) - Photometer/monochromator reflectivity difference too high (20) - High ZA (≥78.5°), low table selection sensitivity (21)

(Continued)

Table 6 (Continued)

4-Byte Word	Comment
	- High ZA, table index limit exceeded (22) - Low ZA (<78.5°), A-B ozone percent difference too large (23) "Good" scans (words 24 through 27), with a distinction between scans when the satellite is ascending and descending (sunlit polar night): - High ZA, descending (24) - Low ZA, descending (25) - High ZA, ascending (26) - Low ZA, ascending (27)
28-37	The following counters have been defined for profile processing: Scans with bad counts, for profile wavelengths only (word 28) Scans for which total ozone is not available (word 29) Total number of scans for which good profile could not be calculated (word 30): - Abnormal reflectivity (31) - Sigma out of range (32) - C out of range (33) - Unacceptable initial residual (34) - Unassigned (35) - Anomalous pressure at which cumulative ozone is one half of total ozone (36) - Excessive solution mixing ratio (37)

Table 7

Format of Trailer File Record*

4-Byte Words	Description
1	Block identifier
2	Trailer file identifier (-1.0)
3	Orbit number of last orbit on tape
4	Day of last scan on tape
5	GMT of last scan on tape
6	Subsatellite latitude of last scan (degrees)
7	Subsatellite longitude of last scan (degrees)
8	Number of tape read errors
9	Number of scans read from RUT tapes
10	Number of scans written on this tape
11-25	Total-ozone processing counters
26-37	Profile processing counters
38	Number of files on tape
	(Continued)

---

*Word 1 contains hexadecimal data, and words 41 onward contain EBCDIC data as indicated. The remaining words are in IBM floating-point format.

Table 7 (Continued)

4-BYTE Word	Description
39	Number of RUT tapes read
40	Spare
41-42	YYDDD for first input tape (EBCDIC)
43-44	YYDDD for second input tape (EBCDIC)
	YYDDD for last (Nth) input tape (EBCDIC)
41+2*N	Start orbit number
42+*N	End orbit number RUT IPD history (16 R*4 words for each input tape) (EBCDIC)
-207	Spare

Detailed Description of Trailer File Record

Word	Comment
11-25	The following counters have been defined for total ozone processing: Total number of scans written on the tape unprocessed (word 11): - For zenith angle too large (12) - Bad counts (14)

(Continued)

Table 7 (Continued)

Word	Comment
	Total number of scans written with negative best ozone (word 15): - For ozone too low/high (16) - For monochromator out of range (17) - Photometer/monochromator reflectivity difference too high (18) - High ZA (≥78.5°), low table selection sensitivity (19) - High ZA, table index limit exceeded (20) - Low ZA (≤78.5°), A-B ozone percent difference too large (21) "Good" scans (words 22 through 25), with a distinction between scans when the satellite is ascending and descending (sunlit polar night): - High ZA, descending (22) - Low ZA, descending (23) - High ZA, ascending (24) - Low ZA, ascending (25)
26-37	The following counters have been defined for profile processing: Scans with bad counts, for profile wavelengths only (word 26) Scans for which total ozone is not available (word 27) Total number of scans for which good profile could not be calculated (word 28): - Abnormal reflectivity (29) - Sigma out of range (30) (Continued)

Table 7 (Continued)

Word	Comment
	- C out of range (31) - Unacceptable initial residual (32) - Unassigned (33) - Anomalous pressure at which cumulative ozone is one half of total ozone (34) - Excessive solution mixing ratio (35) - Spares (-999) (36,37)

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APPENDIX A

F_2' CORRECTION FUNCTION

The F_2' function used for finding the albedos is a function of the orbit number, n. For the 12 monochromator wavelengths and for orbits $n \le 125$, F_2' is given by:

$$F_2'(n) = 1.0 + \frac{(n-100)}{25}(0.011)$$

For orbits $125 < n \le 150$, F_2' is given by:

$$F_2'(n) = 1.011 + \frac{(n-125)}{25}(0.008)$$

For orbits $150 < n \le 175$, F_2' is given by:

$$F_2'(n) = 1.019 + \frac{(n-150)}{25}(0.006)$$

For orbits $175 < n \le 198$, F_2' is given by:

$$F_2'(n) = 1.025 + \frac{(n-175)}{23}(0.002)$$

For orbits $n > 198$, F_2' is given by:

$$F_2'(n) = A_0 + A_1 n + A_2 n^2 + A_3 n^3 + A_4 n^4$$

using the coefficients given in the Table A-1.

Table A-1

F_2' Correction Function

Vacuum Wavelength (nm)	A_0	A_1	A_2	A_3	A_4
255.652	1.016	1.257×10^{-4}	-6.36×10^{-8}	15.60×10^{-12}	-14.28×10^{-16}
273.608	1.015	1.002×10^{-4}	-5.14×10^{-8}	12.82×10^{-12}	-11.85×10^{-16}
283.099	1.015	1.009×10^{-4}	-5.11×10^{-8}	12.37×10^{-12}	-11.23×10^{-16}
287.702	1.013	1.008×10^{-4}	-5.12×10^{-8}	12.39×10^{-12}	-11.22×10^{-16}
292.289	1.011	1.057×10^{-4}	-5.42×10^{-8}	13.03×10^{-12}	-11.71×10^{-16}
297.586	1.012	1.049×10^{-4}	-5.46×10^{-8}	13.27×10^{-12}	-12.02×10^{-16}
301.972	1.011	1.083×10^{-4}	-5.73×10^{-8}	13.96×10^{-12}	-12.67×10^{-16}
305.872	1.012	1.041×10^{-4}	-5.47×10^{-8}	13.31×10^{-12}	-12.06×10^{-16}
312.565	1.011	1.028×10^{-4}	-5.44×10^{-8}	13.14×10^{-12}	-11.81×10^{-16}
317.561	1.013	0.988×10^{-4}	-5.18×10^{-8}	12.38×10^{-12}	-11.09×10^{-16}
331.261	1.013	0.933×10^{-4}	-5.04×10^{-8}	12.27×10^{-12}	-11.08×10^{-16}
339.892	1.012	0.948×10^{-4}	-5.16×10^{-8}	12.42×10^{-12}	-11.03×10^{-16}

A separate F_2' function is used for the photometer. For orbits $n \leq 198$, F_2' n is given by:

$$F_2'(n) = 1.0$$

For orbits $198 < n \leq 600$, F_2' is given by:

$$F_2'(n) = 1.029 - 1.67 \times 10^{-4} n + 1.628 \times 10^{-7} n^2$$

For orbits $600 < n \leq 1308$, F_2' is given by:

$$F_2'(n) = 1.024 - 7.93 \times 10^{-5} n + 6.18 \times 10^{-8} n^2$$

For orbits $n > 1308$, F_2' is given by:

$$F_2'(n) = \frac{974.3}{1027.3 - 5.516 \times 10^{-2} n - 9.72 \times 10^{-7} n^2}$$

APPENDIX B

SAMPLE FORTRAN PROGRAM AND JCL FOR THE OZONE-S TAPE

```
C SAMPLE FORTRAN PROGRAM FOR READING THE OZONE-S TAPE ON THE GSFC
C 360/91 OR 360/75
C
      REAL*8  TAPEIN
      DIMENSION BUFFER(207)
      DIMENSION OZ(12), STDV(12)
      NAMELIST/LIST/ TAPEIN,IFILIN,IFILEN
C
C**** READ THE NAMELIST VARIABLES FROM UNIT 5. TAPEIN = TAPE NAME,
C       IFILIN = FIRST FILE NUMBER DESIRED, IFILEN = LAST FILE DESIRED
    5 READ(5,LIST,END=999)
C**** MOUNT THE TAPE ON UNIT 10
      CALL MOUNT(1,10,TAPEIN,1)
C
C**** READ FROM FILE IFILIN TO IFILEN
      DO 100 IFILE=IFILIN,IFILEN
      IF(IFILE.GE.2) CALL POSN(1,10,IFILE)
C
   10 CONTINUE
C**** READ ONE LOGICAL RECORD FROM UNIT 10
      CALL FREAD(BUFFER,10,LEN,&900,&900)
C
C**** CHECK LOGICAL SEQUENCE NUMBER
C  **** HEADER RECORD (FIRST RECORD ON DATA FILE) FOUND,
C       FIND THE ORBIT NUMBER (ORBN) AND THE YEAR, THEN
C       READ THE NEXT LOGICAL RECORD.
      IF(BUFFER(2) .NE. 1.) GO TO 20
      ORBN=BUFFER(3)
      YEAR=BUFFER(10)
      GO TO 10
C  **** TRAILER RECORD (LAST RECORD ON DATA FILE) FOUND, GO
C       TO NEXT FILE.
   20 IF(BUFFER(2) .LT. -1.) GO TO 100
C  **** TRAILER FILE RECORD FOUND, READ NEXT NAMELIST STEP, STOP
C       IF NO MORE NAMELIST STEPS.
        IF(BUFFER(2) .EQ. -1.) GO TO 200
C
C  **************** DATA RECORDS **********************
C
C**** CHECK ERROR FLAG
      IF(BUFFER(40).LT.0.0) GO TO 10
C
C  **** LATITUDE, LONGITUDE AND SOLAR ZENITH ANGLE IN DEGREES
      XLAT=BUFFER(8)
      XLONG=BUFFER(9)
      ZA=BUFFER(10)
C  **** JULIAN DAY NUMBER
      IDAY=BUFFER(4)
C*************************************************************************
```

```
C    NON THIR DATA (DETERMINED USING REFL. PRESSURE)
C   **** BEST TOTAL OZONE (DOBSON UNITS)
      OZONE=BUFFER(35)
C   **** A-PAIR, B-PAIR OZONE (DOBSON UNITS)
      OZONEA = BUFFER(27)
      OZONEB = BUFFER(31)
C   **** BEST REFLECTIVITY (PER CENT)
      REFL=BUFFER(38)*100.0
C   **** PRESSURE DETERMINED FROM REFLECTIVITY (ATM)
      PRES=BUFFER(37)
C   **** ERROR FLAG
      IERR=BUFFER(40)
C***************************************************************************
C    THIR DERIVED DATA
C   **** BEST THIR OZONE (DOBSON UNITS)
      OZTHIR=BUFFER(21)
C   **** THIR PRESSURE (ATM)
      PTHIR=BUFFER(23)
C   **** THIR REFLECTIVITY (PER CENT)
      RTHIR=BUFFER(24)*100.0
C   **** THIR PERCENT CLOUDINESS
      PRCNT=BUFFER(25)
C   **** THIR TOTAL OZONE ERROR FLAG
      IRTHIR=BUFFER(26)
C***************************************************************************
C    PROFILE DATA
C   **** OZONE AMOUNTS AND STANDARD DEVIATIONS (D.U.) IN 12 LAYERS
      DO 40 I=1,12
      OZ(I)=BUFFER(I+131)
   40 STDV(I)=BUFFER(I+143)
C   **** PROFILE ERROR FLAG
      IPFLAG=BUFFER(176)
C***************************************************************************
C
      GO TO 10
C
  900 CONTINUE
  100 CONTINUE
  200 CONTINUE
C
      GO TO 5
  999 STOP
      END
```

```
//ZMDGGSBU JOB (F12345678D,T,L00001,H00H00)
//*OZONE-S  JCL
// EXEC FORTRANG
//SYSIN DD DISP=SHR,DSN=ZMDGG.PROGRAM.FORT
// EXEC LINKGO,REGION.GO=200K
//GO.FT06F001 DD SYSOUT=A
//GO.FT10F001 DD DISP=(OLD,PASS),UNIT=(6250,,DEFER),
// LABEL=(,NL),VOL=SER=WONG,
// DCB=(RECFM=FB,LRECL=828,BLKSIZE=16560,BUFNO=1)
//GO.DATA5 DD *,DCB=BLKSIZE=3200
 &LIST TAPEIN='SBUV54',IFILIN=2,IFILEN=300, &END
 &LIST TAPEIN='SBUV55',IFILIN=2,IFILEN=500, &END
// EXEC NOTIFYTS
/*
//
```

APPENDIX C

Data Availability and Cost

SBUV Ozone-S data tapes are archived and available from the National Space Science Data Center (NSSDC). The NSSDC will furnish limited quantities of data to qualified users without charge. The NSSDC may establish a nominal charge for production and dissemination if a large volume of data is requested. Whenever a charge is required, a cost estimate will be provided to the user prior to filling the data request.

Domestic requests for data should be addressed to:

National Space Science Data Center
Code 601
NASA/Goddard Space Flight Center
Greenbelt, MD 20771

All requests from foreign researchers must be specifically addressed to:

Director, World Data Center A for Rockets and Satellites
Code 601
NASA/Goddard Space Flight Center
Greenbelt, MD 20771 USA

When ordering data from either NSSDC or the World Data Center, a user should specify why the data are needed, the subject of his work, the name of the organization with which he is connected, and any government contracts he may have for performing his study. Each request should specify the experiment data desired, the time period of interest, plus any other information that would facilitate the handling of the data request.

A user requesting data on magnetic tapes should provide additional information concerning the plans for using the data, i.e. what computers and operating systems will be used. In this context, the NSSDC is compiling a library of routines that can unpack or transform the contents of many of the data sets into formats that are appropriate for the user's computer. NSSDC will provide, upon request, information concerning its services.

When requesting data on magnetic tape, the user must specify whether he will supply new tapes prior to the processing, or return the original NSSDC tapes after the data have been copied.

Data product order forms may be obtained from NSSDC/World Data Center A.

APPENDIX D

SBUV Ozone-S Tape Catalog
First Year

Week Number	Orbit Range(1)	Day Range(2)	Number of Files(3)
01	102-162	304-308	62
02	163-258	309-315	94
03	259-355	316-322	80
04	356-452	323-329	85
05	453-549	330-336	85
06	564-645	338-343	70
07	647-742	344-350	71
08	743-825	351-356	85
09	841-936	358-364	82
10	950-1032	365-006	71
11	1034-1130	007-013	86
12	1131-1213	014-020	66
13	1228-1323	021-027	88
14	1324-1420	028-034	99
15	1421-1517	035-041	85
16	1518-1614	042-048	70
17	1617-1710	049-055	80
18	1711-1807	056-062	92
19	1808-1904	063-069	67
20	1905-1986	070-075	81
21	2003-2097	077-083	77
22	2101-2194	084-090	85
23	2196-2291	091-097	96

(1) See the data inventory in the "User's Guide for the SBUV and TOMS First Year RUT-S and RUT-T Data Sets" for orbit availability for each day.

(2) The data set begins on 10/31/78 (day 304) and ends on 11/3/79 (day 307). Data on the tapes is grouped into days based on the starting time of the orbits. Therefore, minor variations in day ranges may be noted as compared to the data inventory (see the "User's Guide for the SBUV and TOMS First Year RUT-S and RUT-T Data Sets) which groups orbits into days based on the ending time of the orbits.

(3) Number of files includes the header and trailer files plus one file for each orbit present.

SBUV Ozone-S Tape Catalog
First Year (continued)

Week Number	Orbit Range	Day Range	Number of Files
24	2292-2374	098-103	85
25	2389-2484	105-111	97
26	2500-2580	113-118	61
27	2582-2678	119-125	74
28	2679-2775	126-132	81
29	2776-2871	133-139	82
30	2886-2968	141-146	84
31	2969-3065	147-153	61
32	3066-3148	154-159	68
33	3163-3258	161-167	82
34	3273-3355	169-174	50
35	3357-3452	175-181	63
36	3453-3535	182-187	70
37	3550-3645	189-195	81
38	3646-3742	196-202	74
39	3743-3839	203-209	56
40	3840-3922	210-215	72
41	3937-4032	217-223	78
42	4047-4129	225-230	57
43	4131-4226	231-237	69
44	4227-4322	238-244	74
45	4324-4419	245-251	78
46	4455-4514	254-258	47
47	4520-4584	259-263	52
48	4614-4710	266-272	83
49	4711-4805	273-279	73
50	4821-4902	281-286	69
51	4904-4997	287-293	53
52	5001-5096	294-300	82
53	5097-5193	301-307*	97

*Last orbit ends on day 308, 11/4/79.

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15. Supplementary Notes

16. Abstract

Total-ozone and ozone vertical profile results for Solar Backscattered Ultraviolet/Total Ozone Mapping Spectrometer (SBUV/TOMS) Nimbus 7 operation from November 1978 to November 1979 are available. The algorithms used have been thoroughly tested, the instrument performance has been examined in detail, and the ozone results have been compared with Dobson, Umkehr, balloon, and rocket observations. The accuracy and precision of the satellite ozone data are good to at least within the ability of the ground truth to check and are self-consistent to within the specifications of the instrument.

The "SBUV User's Guide" describes the SBUV experiment and algorithms used. It also provides detailed information on the data available on computer tape, including how to order tapes from the National Space Science Data Center.

17. Key Words (Selected by Author(s)) Ozone, Total ozone, Ozone Vertical profile, Nimbus 7 SBUV/TOMS, Ultraviolet radiation, Atmospheric ozone		**18. Distribution Statement** STAR Category 47 Unclassified--Unlimited	
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