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ESTIMATION OF TOTAL OZONE FROM SATELLITE MEASUREMENTS OF BACKSCATTERED ULTRAVIOLET EARTH RADIANCE

CARLTON L. MATEER
DONALD F. HEATH
ARLIN J. KRUEGER

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GSFC — GODDARD SPACE FLIGHT CENTER
GREENBELT, MARYLAND

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Carlton L. Mateer

Canadian Meteorological Service, Toronto, Canada

Donald F. Heath and Arlin J. Krueger

Goddard Space Flight Center, Greenbelt, Md., 20771

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Goddard Space Flight Center

Greenbelt, Maryland

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ABSTRACT

Total ozone is estimated from Nimbus IV satellite measurements of the attenuation of backscattered radiances at wavelengths between 3100 and 3400 Å. A measurement of the backscattered radiance at 3800 Å, outside the ozone absorption band, is used to determine an equivalent Lambert albedo for the cloud-ground-haze surface viewed by the instrument. The measured relative attenuation at two wavelengths is compared with such values pre-computed for a series of standard ozone profiles and corrected for the equivalent Lambert albedo. Total ozone is obtained by interpolation. Two alternative methods are used to assign an equivalent Lambert albedo at the absorbing wavelengths. In the first method, the value determined at 3800 Å is assumed to be applicable at the absorbing wavelengths. In the second method, the albedo at the absorbing wavelengths is calculated for a sample of 320 cases of near-coincidence with ground-based Dobson spectrophotometer measurements of total ozone. Regression equations are then developed to predict the absorbing wavelength albedo from the 3800 Å

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albedo. Finally, these regression equations are introduced into the total ozone evaluation procedure. Total ozone values estimated by these methods are compared with the Dobson (ground-truth) data by linear regression. Using either albedo method, the Dobson data are recovered from the satellite data with a standard error of estimate of about 0.020 atm-cm from measurements at 3125 and 3312 Å, and with a standard error of about 0.025 atm-cm from measurement 3175 and 3398 Å. Part of this error may be attributed to a lack of perfect simultaneity in space and time between the Dobson and satellite data. The available evidence suggests that the true standard error of the satellite data may be 0.015 atm-cm or less for solar zenith angle less than sixty degrees.

ESTIMATION OF TOTAL OZONE FROM SATELLITE MEASUREMENTS OF BACKSCATTERED ULTRAVIOLET EARTH RADIANCE

1. Introduction

Backscattered ultraviolet earth radiances have been measured from Nimbus IV by means of a double monochromator that is stepped every 32 seconds through 12 discrete wavelengths between 2500 and 3400 Å in the Hartley-Huggins ozone absorption band. The monochromator has a 10 Å bandpass and views the earth in the satellite's nadir direction. Once per orbit, near the northern terminator, a ground-aluminum diffuser plate is deployed to measure the extra-terrestrial solar irradiance. A separate filter photometer, with a 50 Å band-pass and with the same field of view as the monochromator measures the back-scattered earth radiance at 3800 Å, outside the ozone absorption band. Further details of the instrument package may be found in The Nimbus IV User's Guide.

The physical basis for estimating total ozone from backscattered ultraviolet radiances has been discussed by Dave and Mateer (1967). It will suffice to say here that total ozone is inferred from measurements at wavelengths near the long-wavelength end of the ozone absorption band. At these wavelengths, the absorption is sufficiently weak so that most of the photons reaching the satellite instrument have passed through the ozone layer and been backscattered from within the troposphere. Thus, the backscattered radiance at the satellite depends on (i) the attenuation of the direct solar beam on its slant path through the ozone layer, (ii) the reflecting power of the troposphere (molecular and aerosol scattering and surface and cloud reflections), and (iii) the attenuation of the diffusely reflected photon stream as it passes vertically upward through the ozone layer. If θ_0 is the sun's zenith angle for the solar ray incident on the earth's surface at the sub-satellite point and θ is the sun's zenith angle for the same ray at the level of maximum ozone density (about 22 km), then the total attenuation path of backscattered photons through the ozone layer, from (i) and (iii) is proportional to $1 + \sec \theta$.

The reflecting power of the troposphere is highly variable. For surface-based total ozone determinations, measurements are made at a pair of wavelengths, one fairly strongly absorbed by ozone, the other rather weakly absorbed. The two wavelengths are separated by approximately 200 Å so that scattering effects are about the same at each wavelength and the relative attenuation for the pair is sensitive mostly to total ozone. Dave and Mateer (1967) found this to be true for backscattered radiances, provided absorption at the shorter, more strongly absorbed wavelength, met the criterion for penetration discussed in the preceding paragraph. Accordingly, we infer total ozone from the relative logarithmic attentuation (N) for wavelength pairs: E - 3125, 3312 Å and F - 3175, 3398Å. For example

$$N\,(3125,\ 3312) = \log_{10}\{F_0/I\}_{3125} - \log_{10}\{F_0/I\}_{3312} \qquad (1)$$

where F_0 = extraterrestrial solar irradiance, and

I = backscattered earth radiance.

The measured value of N is compared with values pre-computed for a series of different standard ozone profiles and total ozone is estimated by interpolation.

2. Evaluation procedure

The pre-computed data cover the full range of possible solar zenith angles ($0 \leq \theta_0 \leq 90°$) and all orders of molecular scattering are accounted for by successive iteration of the auxiliary equation (Dave, 1964) in a pseudo-spherical atmosphere (De Luisi and Mateer, 1971). The computations were carried out for 16 standard ozone profiles, including three in a low-latitude series (latitude less than 25°), six in a mid-latitude series, and seven in a high-latitude series (latitude greater than 50°). The profiles corresponding to the lowest and highest total ozone amounts for each series are shown in Figure 1. The low-latitude profiles were developed from data obtained by direct soundings at the Canal Zone (Hering and Borden, 1965); the mid-latitude profiles from direct soundings at Boulder, Colorado (Dütsch, 1966); and the high-latitude profiles from direct soundings at Resolute, Canada (data obtained in advance of publication). Two sets of tables were computed, one for a surface pressure of 1.0 atm, the other for 0.4 atm.

Perhaps the most critical aspect of the evaluation method is the treatment of cloud and surface reflections and backscattering by tropospheric aerosols. In our method, the areal average of these effects is incorporated into the procedure as an equivalent (Lambert) surface albedo or reflectivity (R). For a given wavelength, we may write

$$I\{\Omega, \theta_0, R\} = I\{\Omega, \theta_0, 0\} + T\{\Omega, \theta_0\} \cdot R/(1 - R \cdot S\{\Omega\}) \tag{2}$$

where

Ω = total ozone for a standard profile

$I\{\Omega, \theta_0, R\}$ = backscattered radiance for conditions specified by Ω, θ_0, R,

$I\{\Omega, \theta_0, 0\}$ = backscattered radiance for conditions specified by Ω, θ_0, and $R = 0$,

$T\{\Omega, \theta_0\}$ = extraterrestrial irradiance times direct plus diffuse incoming transmittance times outbound diffuse transmittance. In Dave's (1964) notation, T is I*/Q.

$S\{\Omega\}$ = fractional whole-atmosphere backscattering for isotropically reflected surface radiation, $S^b(\tau_1)$ in Dave's notation.

In the case of photometer measurements at 3800 Å outside the ozone absorption band, the Ω-dependence drops out of all terms in Eq. (2), and the measurement of $I\{\theta_0, R\}$ permits the direct calculation of R,

$$R = \frac{I\{\theta_0, R\} - I\{\theta_0, 0\}}{T\{\theta_0\} + S[I\{\theta_0 R\} - I\{\theta_0, 0\}]} \tag{3}$$

In the tables, the quantities $I\{\Omega, \theta_0, 0\}$ and $T\{\Omega, \theta_0\}$ are listed for each absorbing wavelength, each total ozone, and each solar zenith angle, while $S\{\Omega\}$ is listed for each absorbing wavelength and each total ozone. Similar listings apply for 3800 Å, but without the total ozone dependence.

For the approximately 2-second dwell time at each monochromator wavelength setting, simultaneous averages of the backscattered radiance for the monochromator and for the photometer are obtained. The non-measured quantities in Eq. (3) are obtained from the 3800 Å tables by logarithmic interpolation with respect to total relative path (1 + sec θ) and R is calculated. The simplest approach is to assume that R (3800) is also applicable at the shorter absorbing wavelength. Accordingly, using a series of values of Ω (optimized search routine), values of $I\{\Omega, \theta_0, R\}$ are computed by Eq. (2) (using logarithmic interpolation re (1 + sec θ) where necessary) for each absorbing wavelength, and values of N are computed from Eq. (1). A value of N is also computed for the observed radiances and the search is continued until computed values of N are obtained just above and below this observed value. Total ozone is obtained by linear interpolation. In this way, four total ozone estimates are derived: one for each of the two wavelength pairs, in turn, for each of the two surface pressure tables. A simple ad hoc procedure is used to estimate a final value for each wavelength pair, viz., for $R \leq 0.2$, the value obtained with the 1 atm surface pressure table is taken; for $R \geq 0.8$, the value obtained with the 0.4 atm table is selected; and, for intermediate R, a linear combination of the two values is computed (so-called tea-mixing rule).

At large values of total relative path, when the sun is not far from the horizon, the backscattered radiance at 3125 Å no longer meets the penetration criterion discussed earlier, and the measurements for the 3125, 3312 Å pair lose sensitivity to total ozone. Since the sensitivity depends both on path length and total ozone, we calculate an interpolation sensitivity (essentially $\delta N / \delta \Omega$) for each determination and the final "best" value is selected as that for the wavelength pair having the greater sensitivity.

3. Results

Total ozone values have been obtained by the above method for the period April 10 to July 13, 1970. From these data, we have obtained a sample of 320 approximate coincidences of satellite data with Dobson spectrophotometer "ground-truth" measurements. For the E wavelength pair (3125, 3312), the satellite data average 0.024 atm-cm too low and, for the F wavelength pair (3175, 3398), 0.020-atm-cm too low. If we seek a simple linear regression between the Dobson and satellite data, we find

$$\hat{\Omega} = 0.0466 + 0.9290\, \Omega_E$$
$$\hat{\Omega} = 0.0589 + 0.8802\, \Omega_F \qquad (4)$$

where $\hat{\Omega}$, Ω_E, Ω_F are the estimated Dobson, satellite E pair, and satellite F pair total ozone values, respectively. After application of Eq. (4) to the (dependent) sample, the standard errors of estimate are 0.020 and 0.025 atm-cm, respectively, in absolute units, and 5.6 and 7.3, respectively, as percentages.

As indicated earlier, the treatment of equivalent surface albedo is a critical feature of the evaluation procedure. It is of interest, therefore, to examine the wavelength dependence of this albedo. This has been done for the 320 coincidence cases, with total ozone assumed known, by using the Ω-dependent form of Eq. (3) to calculate R for each absorbing wavelength. Quadratic regression relationships between calculated albedo and that at 3800 Å are shown in Fig. 2 for 3125 and 3312 Å. The important feature of these curves for total ozone estimation is that the equivalent surface albedo is greater at 3125 than at 3312 for both surface pressure tables. Standard errors for estimating the equivalent surface albedo at the absorbing wavelengths from that obtained at 3800 Å are listed in Table 1 for both linear and quadratic regressions.

The albedo regressions have been introduced into the total ozone evaluation procedure so that the R used in Eq. (2) is the regression value at the absorbing wavelength. With this change, the satellite data average 0.0014 atm-cm too high for the E pair and 0.0008 atm-cm too low for the F pair. Standard errors of estimate are 0.020 and 0.025 atm-cm, respectively, in absolute units, and 5.7 and 7.3 respectively, as percentages. If we perform a linear regression with these new satellite values (Ω'_E, Ω'_F), we find

$$\hat{\Omega} = 0.0269 + 0.9186\,\Omega'_E$$
$$\hat{\Omega} = 0.0443 + 0.8737\,\Omega'_F \qquad (5)$$

In absolute units, the standard errors of estimate are reduced trivially to 0.019 and 0.024 atm-cm, respectively. According to Eq. (5), the satellite values average a little too low at low total ozone and a little too high at high total ozone. Results for the E pair are shown in Fig. 3, the dashed lines being one standard error of estimate from the regression line. It is not surprising that Eqs. (5) are not significantly better than Eq. (4). Evidently, the non-linearities involved in Eq. (2) and in the interpolation are not sufficiently pronounced compared to the random differences exhibited in Fig. 3 to permit a significant improvement.

4. Discussion

The true standard error of the satellite-derived total ozone data is probably somewhat less than the errors calculated above. First, the coincidence in time and space between the satellite and ground truth is never perfect. Second, the satellite gives us some sort of weighted areal average, whereas the Dobson value is integrated along the slant path between the instrument and the sun. A crude measure of the extent of the non-coincidence between the satellite and Dobson values may be inferred from Table 1. At 3398 Å, where the absorption effect is quite small, the standard error is roughly one-half the value at 3125 Å, where the absorption effect is substantial. Since there is no good a priori reason for instrumental errors to be larger at 3125 than at 3398, this is precisely the kind of effect we should observe as a result of imperfect coincidence. This argument is not completely conclusive, because the greater standard error at 3125 may be attributed in part to differences between the standard ozone profile and that actually existing in the atmosphere at the time of a satellite observation.

However, Dave and Mateer (1967) have shown that errors due to profile differences are probably quite small for high sun and, since fewer than 20 of our near-coincidence sample apply to solar zenith angles in excess of 60°, it is probable that the true standard error of the satellite total ozone data is approximately 0.015 atm-cm or less, at high sun.

Future work will be aimed at increasing the size of the inter-comparison sample which, for the northern hemisphere winter, will include many more low-sun data, and at testing the evaluation procedure using dependent and independent samples. In addition, improvement of the overall procedure by means of stratification of the data sample by latitude, solar zenith angle, albedo, etc., will be investigated, as will the ad hoc pressure interpolation.

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Table 1

Standard Errors for Estimating Equivalent Surface Albedo

at Absorbing Wavelengths from Value at 3800 Å

Surface Pressure (atm)	Wavelength (Å)	Linear Regression Error	Quadratic Regression Error
1.0	3125	0.082	0.081
	3175	0.057	0.056
	3312	0.044	0.043
	3398	0.038	0.038
0.4	3125	0.060	0.057
	3175	0.046	0.044
	3312	0.035	0.034
	3398	0.032	0.031

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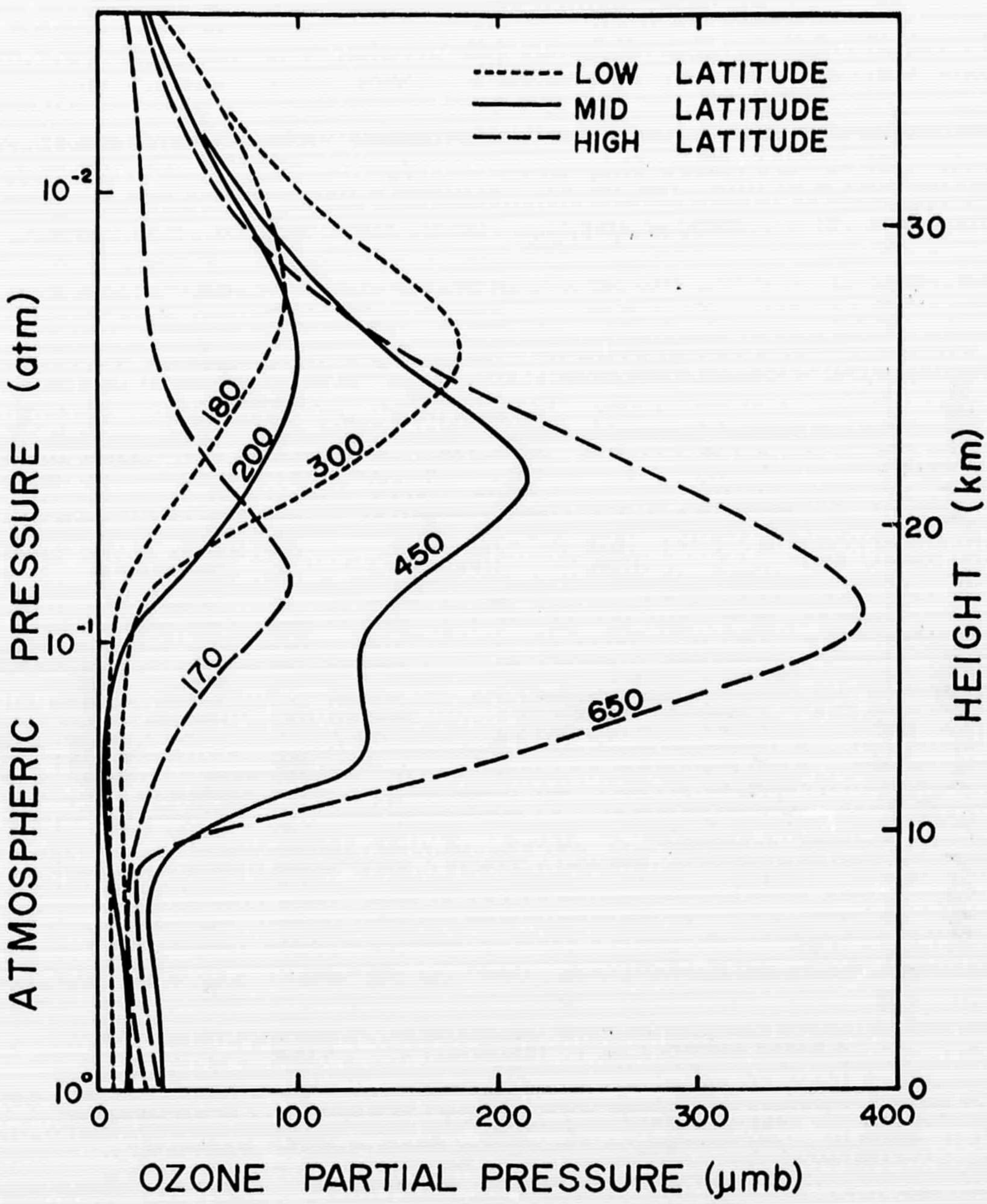

Figure 1. Standard Ozone Profiles for Lowest and Highest Total Ozone for Low-, Mid-, and High-Latitude Series (Total Ozone Applicable to Each Profile is Given in m atm-cm.)

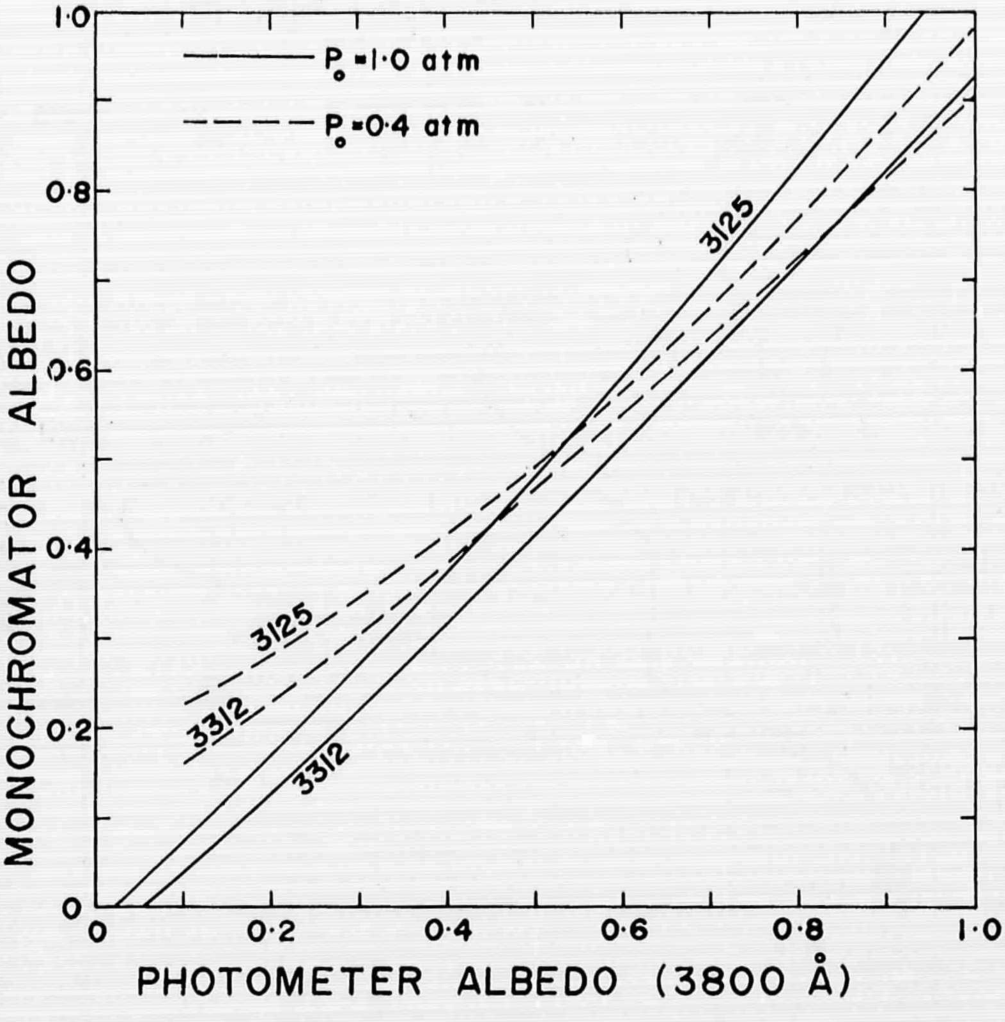

Figure 2. Regression Curves Giving Equivalent Surface Albedo at Absorbing (monochromator) Wavelengths as a Function of Albedo at 3800 Å (Photometer)

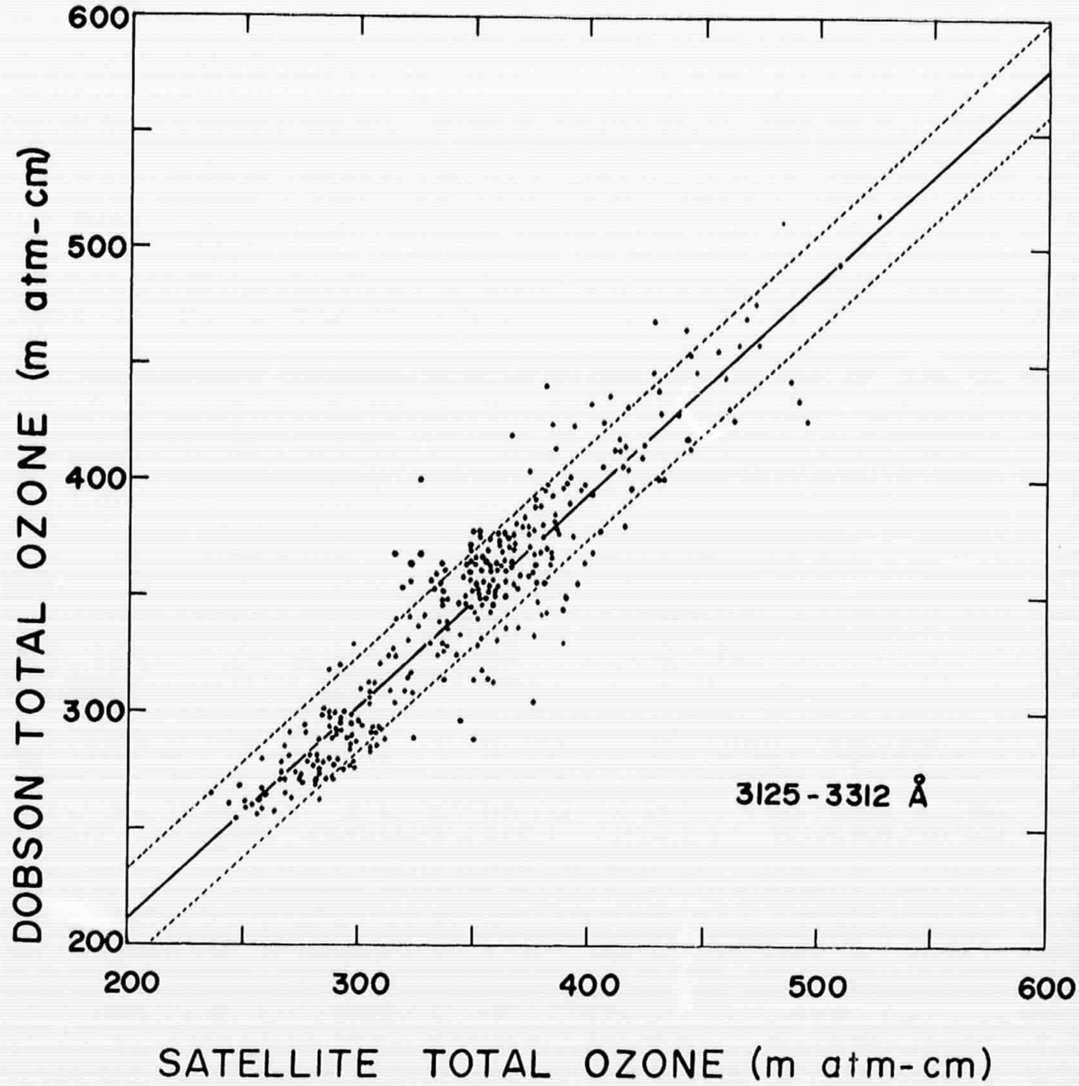

Figure 3. Scatter Diagram Showing Relationship Between Dobson and Satellite Total Ozone for the E Wavelength pair (Dashed lines are one standard error of estimate from linear regression line.)