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Initial Estimate of NOAA-9 SBUV/2 Total Ozone Drift:
Based on Comparison with Re-calibrated TOMS Measurements and Pair Justification of SBUV/2

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Abstract-Newly recalibrated Version 6 TOMS data are used as a reference measurement in a comparison of monthly means of total ozone in 10 degree latitude zones from SBUV/2 and the nadir measurements from TOMS. These comparisons indicate a roughly linear long-term drift in SBUV/2 total ozone relative to TOMS of about 2.5 Dobson units per year at the equator over the first three years of SBUV/2. The pair justification technique is also applied to the SBUV/2 measurements in a manner similar to that used for SBUV and TOMS. The higher solar zenith angles associated with the afternoon orbit of NOAA-9 and the large changes in solar zenith angle associated with its changing equator crossing time degrade the accuracy of the pair justification method relative to its application to SBUV and TOMS, but the results are consistent with the SBUV/2 - TOMS comparisons, and show a roughly linear drift in SBUV/2 of 2.5 - 4.5 Dobson units per year in equatorial ozone.

SBUV/2 - TOMS Comparisons

The first ten years of data (11/78 - 10/88) from the Total Ozone Mapping Spectrometer (TOMS) have been reprocessed using an improved long-term calibration. The calibration adjustment was derived using the pair justification technique. The nadir samples of these data have been averaged to provide cross-track spacial resolution comparable with the SBUV/2 field of view, and then averaged monthly in 10 degree latitude bands centered at the equator. A little over three years (3/85-8/88) of reprocessed SBUV/2 total ozone data have been averaged monthly in the same latitude bands. Figure 1 shows the difference of these monthly zonal means in the equatorial band over the period of the SBUV/2 data set. The standard error of the monthly means contain a lot of seasonal and day-to-day variance. The standard errors of daily means of SBUV/2 and TOMS should be considered later in this study to provide a statistical estimate of the noise in this comparison. For now, it is noted that an apparent seasonal cycle in the differences is resolved to some extent. A mechanism for such a cycle is not well understood at this time, but correlation between this cycle and the variation in the SBUV/2 solar azimuth angle should be studied further. Note that a smaller seasonal cycle of about 1% amplitude is present in the TOMS total ozone relative to SBUV (Wellemeyer et al, 1988), which also correlates with this effect. A least-squares linear fit to the data in Figure 1 gives a drift in SBUV/2 relative to the preliminary V6 TOMS of about 2.4 D.U./Yr. Figure 2 shows changes in SBUV/2 equatorial reflectivity relative to V6 TOMS. Figures 1 and 2 provide somewhat different impressions of the time signature of SBUV/2 -V6 TOMS differences.

Figures 3 and 4 show differences between the monthly zonal means of the A-pair (312.5-331.2 nm) and B-pair (317.5-331.2 nm) total ozone from SBUV/2 and the corresponding pairs from TOMS. These comparisons indicate that the B-pair from SBUV/2 drifts about twice as much relative to V6 TOMS as does the SBUV/2 A-pair. Note that the V6 TOMS data have been pair justified so that the B'-pair (317.5-339.8 nm) actually used in the TOMS retrieval gives the same long-term change in total ozone as does the V6 TOMS A-pair. The difference in drift between the pair results from SBUV/2 are symptomatic of a wavelength dependent calibration error in the albedo measured by SBUV/2. This is because different pairs of total ozone wavelengths have different sensitivities to this type of calibration error. The two major factors in these differences are the sensitivity of the pair to the presence of ozone, and the wavelength separation the pair. The diagram below illustrates that the B-pair is about twice as sensitive to a given error in the N-value than the B-pair.

**Basic Total Ozone Retrieval and Impact of
Pair Sensitivity on Error Budget**

Measure Quantity: $N = -100 \log [I/F]$

Pair N values: $N_A = N_{313} - N_{331}$ $N_B = N_{318} - N_{331}$

For a given set of viewing conditions:

$$\text{A-pair slope} = \frac{\partial N_A}{\partial \Omega}$$

$$\text{B-pair slope} = \frac{\partial N_B}{\partial \Omega}$$
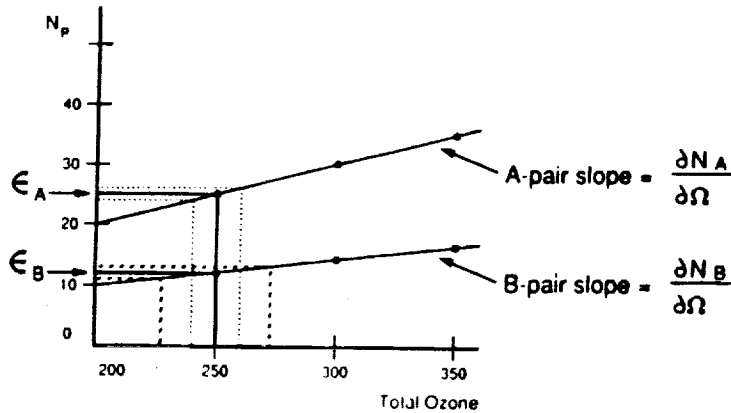
Secondly, if a wavelength dependent error in calibration is present, it would be expected that the size of the error across a given pair would be proportional to its wavelength separation. The table below shows the wavelength separation and the ozone sensitivity of several pairs of total ozone wavelengths. Also shown is the ratio of wavelength separation to ozone sensitivity which provides a sensitivity factor for each pair of wavelengths to the presence of wavelength dependent calibration errors that are proportional to wavelength separation.

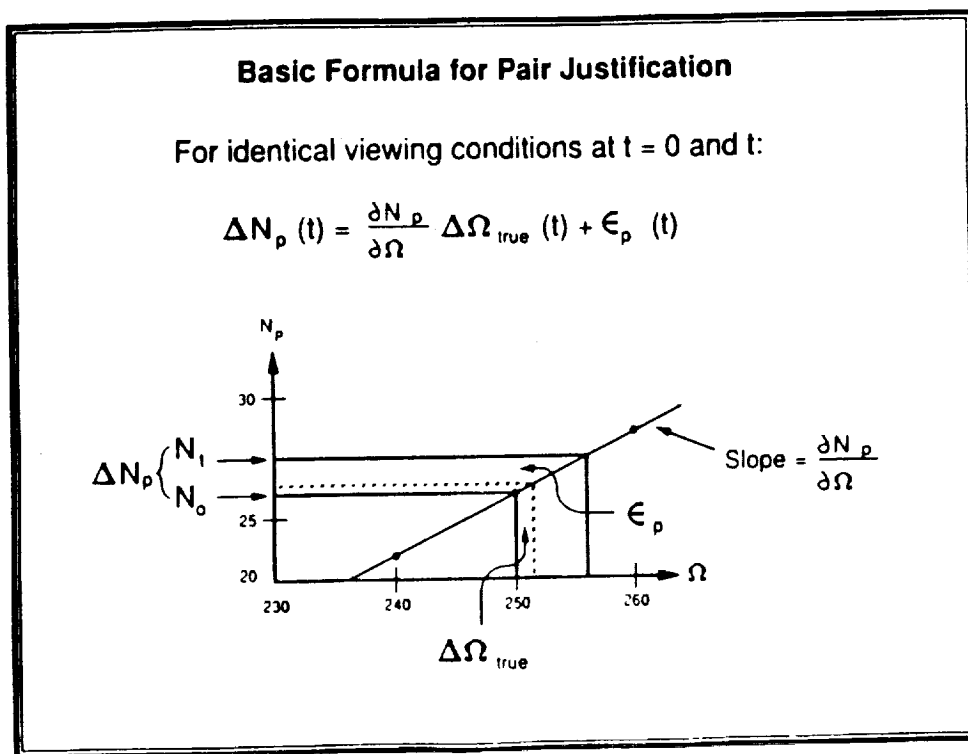Different pairs have different sensitivities to wavelength-dependent calibration errors.

This sensitivity depends on:

1) The separation of the wavelengths used
2) The differential ozone absorption across the pair (ozone sensitivity)

Pair Name	Wavelength (nm)	$\Delta \lambda$ (nm)	Sensitivity (N-value/D.U.)	$\dfrac{\Delta \lambda}{\text{Sensitivity}}$
B'	318 - 340	22.3	0.073	306
B	318 - 331	13.7	0.063	218
A	313 - 331	18.7	0.125	150
A'	313 - 318	5.0	0.062	81
D	306 - 313	6.7	0.190	35

The D-pair retains high ozone sensitivity at a small wavelength separation because it lies on a steeper portion of the Hartley absorption peak than the other pairs. Because of the higher absorption, however, this pair only provides sufficient penetration to measure total ozone at near overhead sun conditions. This pair was used to good advantage in pair justification of the SBUV and TOMS data sets, but cannot be used for SBUV/2 because of the higher solar zenith angles associated with the afternoon equator crossing of NOAA-9. Pair justification can still be applied to SBUV/2, however by coupling other pairs with contrasting sensitivities to wavelength dependent calibration errors and insisting that they give the same measurement of long-term changes in total ozone.

The diagram below illustrates the fundamental formula used in the application of pair justification. For identical viewing conditions at time t=0 and time t, a change in the measured pair N-value is the sum of two terms: the change in N-value due to real changes in ozone, and the change due to drift in instrument calibration. A difficulty in applying this formula to the SBUV/2 data is that viewing conditions are generally quite different at t=0 and t. Figure 5 shows the monthly zonal mean of the solar zenith angles associated with the SBUV/2 total ozone measurements as a function of time. Because of this, a large adjustment (about 11 N-value units for A-pair) must be made to the measured N-values in 8/88 to normalize them to initial conditions. A test of the accuracy of this correction is discussed below.

Basic Formula for Pair Justification

For identical viewing conditions at t = 0 and t:

$$\Delta N_p (t) = \frac{\partial N_p}{\partial \Omega} \Delta \Omega_{true} (t) + \epsilon_p (t)$$

The application of this basic formula consists of writing it for a pair of wavelengths. An assumption about the wavelength dependence of the calibration is required, however to relate the errors of the pairs used. As shown below, this is accomplished by assuming (first order) that the pair error is proportional to the wavelength separation of the pair. This results in a set of three equations with three unknowns (true ozone change, and the errors across the coupled pairs). The solution for true ozone change can be used to compute pair calibration errors across the coupled pairs, and any other total ozone pairs.

Write basic formula for pair of pairs:

$$\Delta N_A (t) = \frac{\partial N_A}{\partial \Omega} \Delta \Omega_{true} (t) + \epsilon_A (t)$$

$$\Delta N_{B'} (t) = \frac{\partial N_B}{\partial \Omega} \Delta \Omega_{true} (t) + \epsilon_B (t)$$

Assume pair error proportional to $\Delta \lambda$:

$$\epsilon_A / \epsilon_{B'} = \Delta \lambda_A / \Delta \lambda_{B'}$$

Solve for $\Delta \Omega_{true} (t)$, $\epsilon_A (t)$, $\epsilon_{B'} (t)$, etc.

In general, this solution can be applied to individual scans. In practice, monthly zonal means of the measured N-values have been used, and monthly solutions to the above equations provide estimates of pair calibration errors. Additionally, the averaged N-values have been de-seasonalized using the three year mean annual cycle as part of the effort to normalize the measured N-values to standard viewing conditions. In such a procedure, the linearity of operations performed in a convenient order come into question. The linearity test described below provides a test of the accuracy of the basic pair justification applied to mean N-values, and of the large solar zenith correction necessitated by precession of the NOAA-9 satellite.

Linearity Test of Basic Equation

Compute measured ozone change using averaged, deseasonalized, adjusted N-value changes:

$$\Delta \Omega_{meas} (t) = \Delta N_p (t) / \frac{\partial N_p}{\partial \Omega}$$

Compare with averaged, deseasonalized ozone from individual retrievals.

This test checks the linearity assumed in computing ozone from averaged deseasonalized N-values and the accuracy of adjustments.

The results of such a test applied to the first ten years of TOMS data are illustrated in Figure 6. The measured ozone changes derived from the individual V5 TOMS total ozone retrievals (averaged and de-seasonalized), and those derived from the averaged, de-seasonalized V5 TOMS N-values are shown as well as their difference. This result indicates that the basic pair justification equation is quite accurate as applied to the TOMS data set. Figure 2 illustrates the results of the same test applied to the SBUV/2 data set. Here, the measured change in equatorial ozone has no systematic long-term changes as seen in the case of TOMS. The difference between the two computations shows both larger variations and a systematic difference that is not present in the TOMS case.

Another possible error source in the pair justification method is related to the assumption of a linear dependence with wavelength of the calibration error. How sensitive are the pair justification results to the possible presence of curvature in the actual wavelength dependence the calibration error? Simulation studies have been performed in an effort to answer this question. The pair justification formulation is applied to simulated N-values that are computed assuming zero "true" ozone change and contain errors of arbitrary wavelength dependence. Figure 8 shows the results of pair justification applied to simulated N-value changes containing error that is linear wavelength. In this case, the simulated errors are consistent with the assumed wavelength dependence, and each alternate coupling of pairs does a perfect job of retrieving that dependence. For the results in Figure 9, however, a second order dependence has been included in the simulated N-value changes. Here, different couplings of pairs exhibit different sensitivities to the presence of curvature in the actual wavelength dependence. This sensitivity depends on the ozone sensitivities of the coupled pairs, and the wavelength range of the combined pairs. Because of the differing sensitivities of alternate couplings of pairs, the divergence of pair justification results from different couplings might be used to diagnose curvature. Because of the high solar zenith angles and associated errors in the basic equation, the applicability of this technique to the SBUV/2 data is limited.

The pair justification has been applied to the monthly averaged, deseasonalized, adjusted N-values measured by the SBUV/2 in the 10 degree equatorial zone using A-B' and A-A' couplings. The A-pair calibration errors derived using this method are shown in Figure 10. The equivalent error in equatorial ozone for the two couplings is shown in Figure 11. Least squares linear regressions applied to these results give slopes (standard errors) of 2.7 (0.2) D.U./Yr. for A-B' and 4.3 (0.4) D.U./Yr. for A-A'. Though the difference in these results appear to be statistically significant, and might indicate the presence of some curvature in the actual wavelength dependence of the calibration error, these differences might also be due to uncertainty in N-value adjustments for increasing solar zenith angles or non-linearities in the averaging process as described above.

Conclusions

The non-local noon equator crossing time and drift in equator crossing time of the NOAA-9 orbit limit the accuracy of the pair justification technique when applied to SBUV/2 data. This is largely due to the fact that the D-pair wavelengths (305.8-312.5 nm) cannot be used at solar zenith angles much larger than 30 degrees. When applied to the SBUV/2 data set, the pair justification method indicates that the drift in equatorial total ozone is between 2.5 and 4.5 D.U./Yr. This estimate is somewhat higher than estimates based on SBUV/2 - V6 TOMS comparisons presented here or SBUV/2 - Dobson comparisons performed elsewhere.

Continued Analysis

Some further work is planned in understanding the uncertainties in the pair justification technique as applied to the NOAA-9 SBUV/2 data set. In particular, the sources of non-linearities and possible errors in the solar zenith angle correction to the measured N-values will be considered. The pair justification technique, however appears to be of limited value when applied to this data set, and alternate means to the correction of the long-term calibration of the NOAA-9 SBUV/2 should be sought.

Further analysis of the SBUV/2 - V6 TOMS total ozone comparisons is planned. The latitude dependence of the long-term drift and the seasonal variation in the bias should provide additional insight to the character of the calibration error in the SBUV/2.
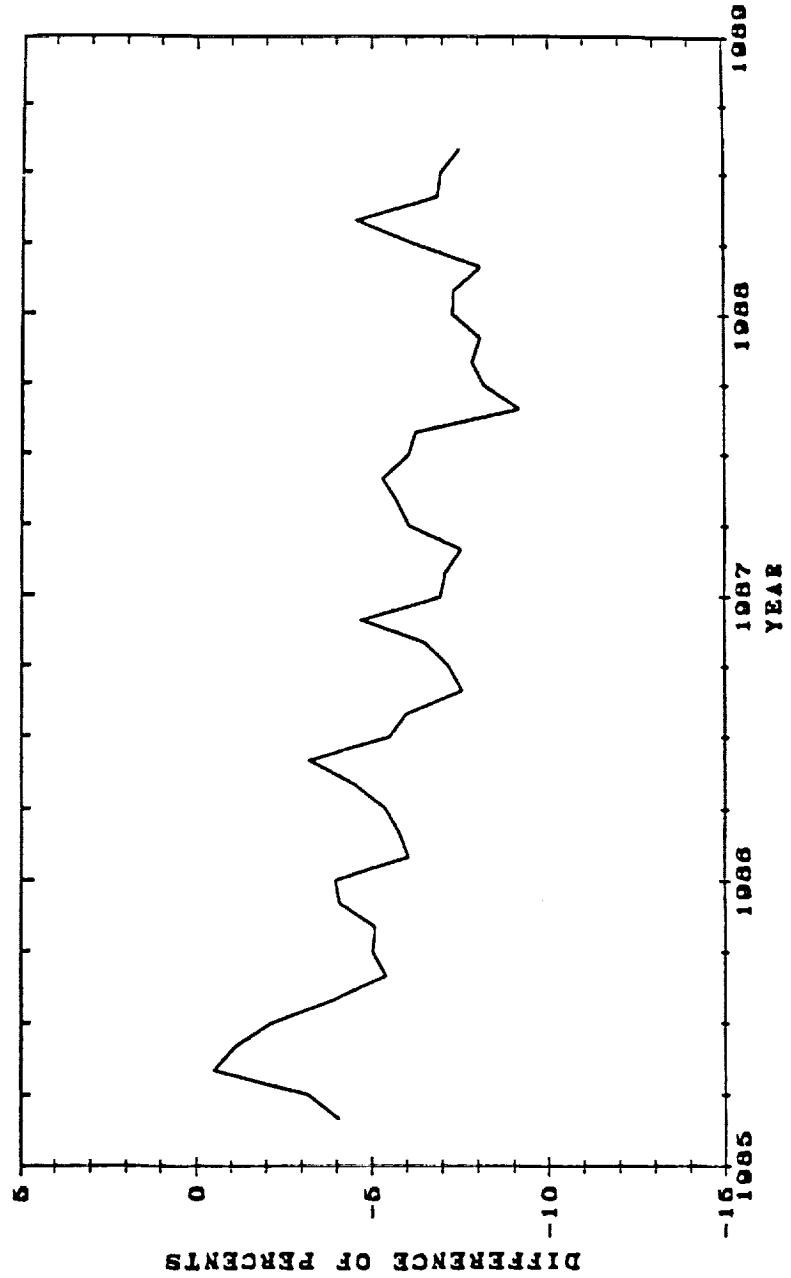
Reference

Wellemeyer, C.G., A.J. Fleig, and P.K. Bhartia; Internal Comparisons of SBUV and TOMS Total Ozone Measurements, Proceedings of the Quadrennial Ozone Symposium 1988, R.D. Bojkov, editor (1989).

Figure 1. Difference of monthly zonal means of total ozone (SBUV/2 - TOMS)
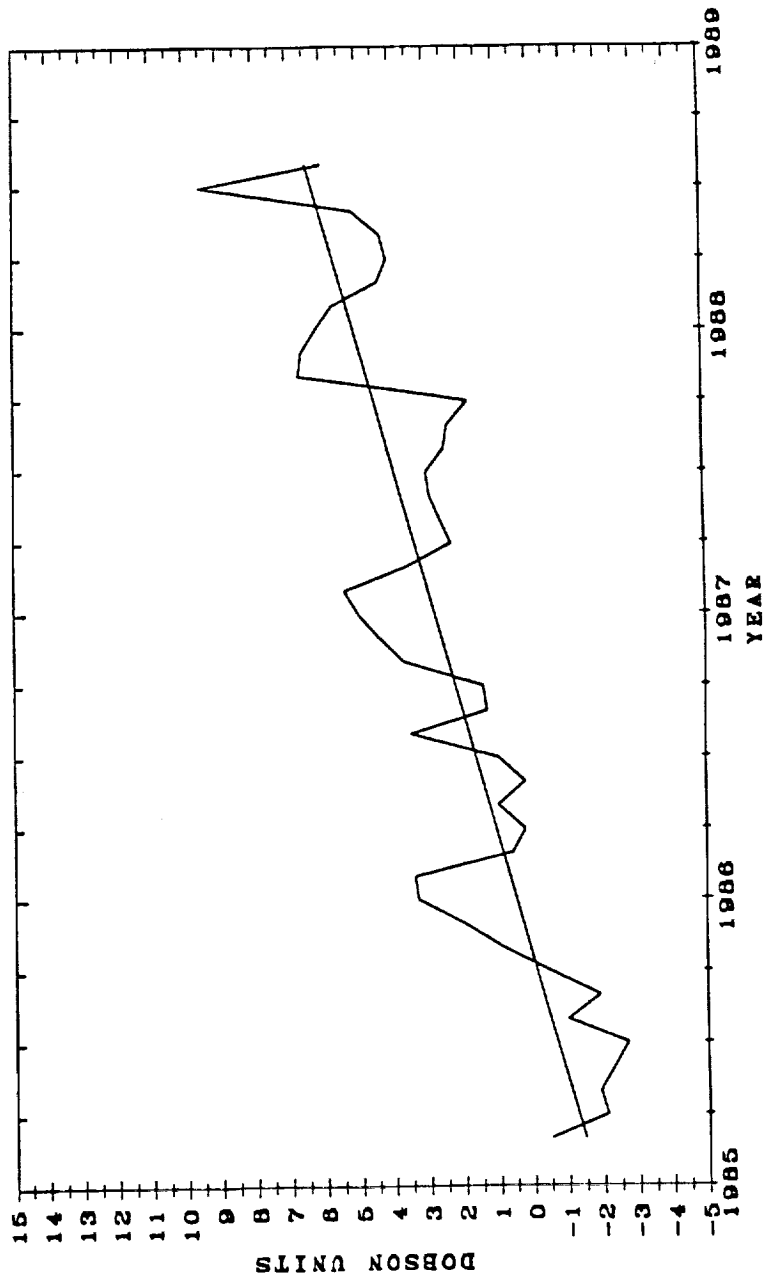
Figure 2. Difference of monthly zonal means of reflectivity (SBUV/2 - TOMS)

Figure 3. Difference of monthly zonal means of A-pair ozone (SBUV/2 - TOMS)
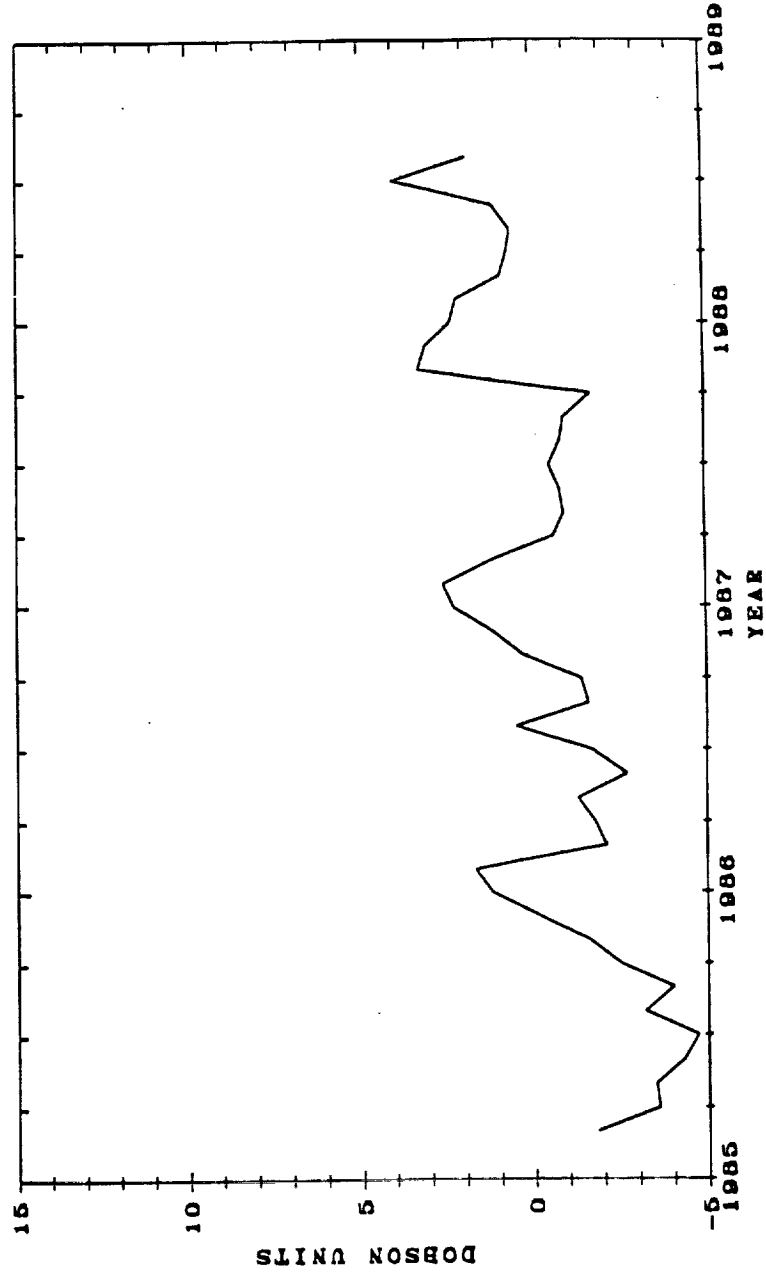
Figure 4. Difference of monthly zonal means of B-pair ozone (SBUV/2 - TOMS)
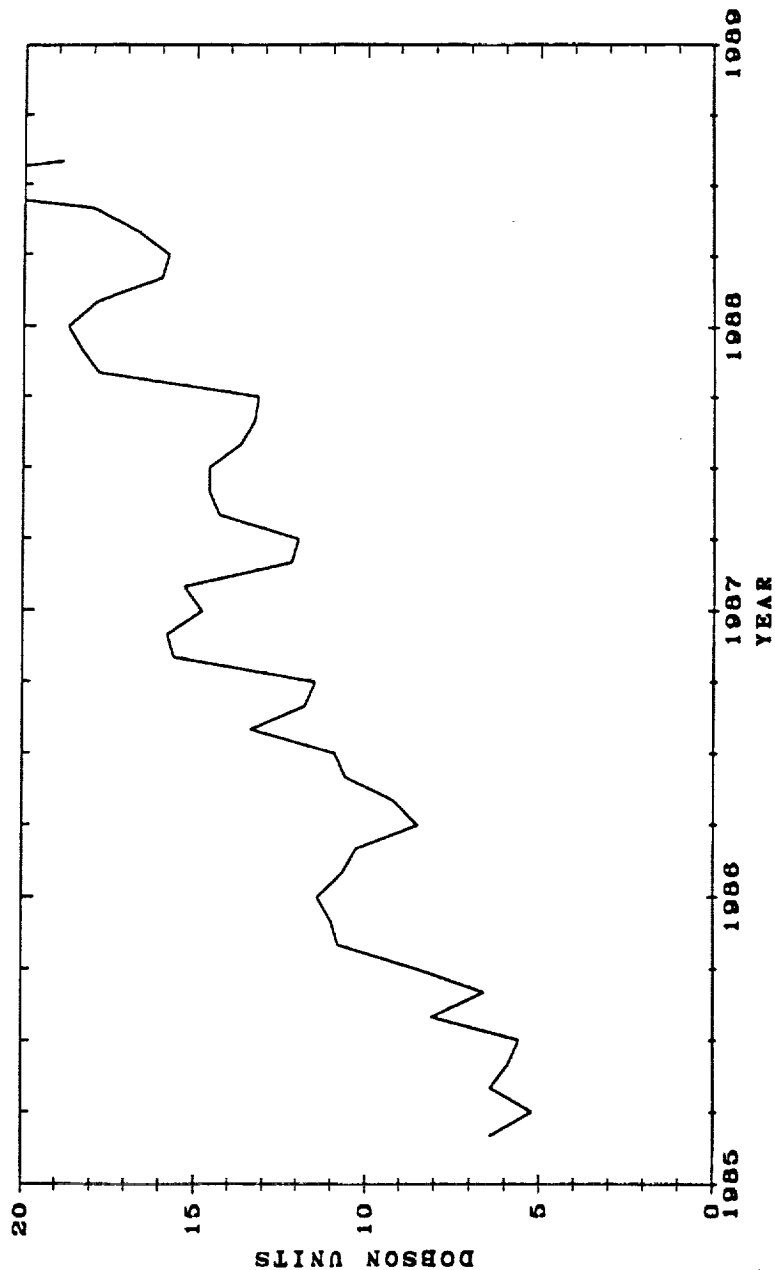
Figure 5. Monthly zonal mean of solar zenith angle at SBUV/2 field of view
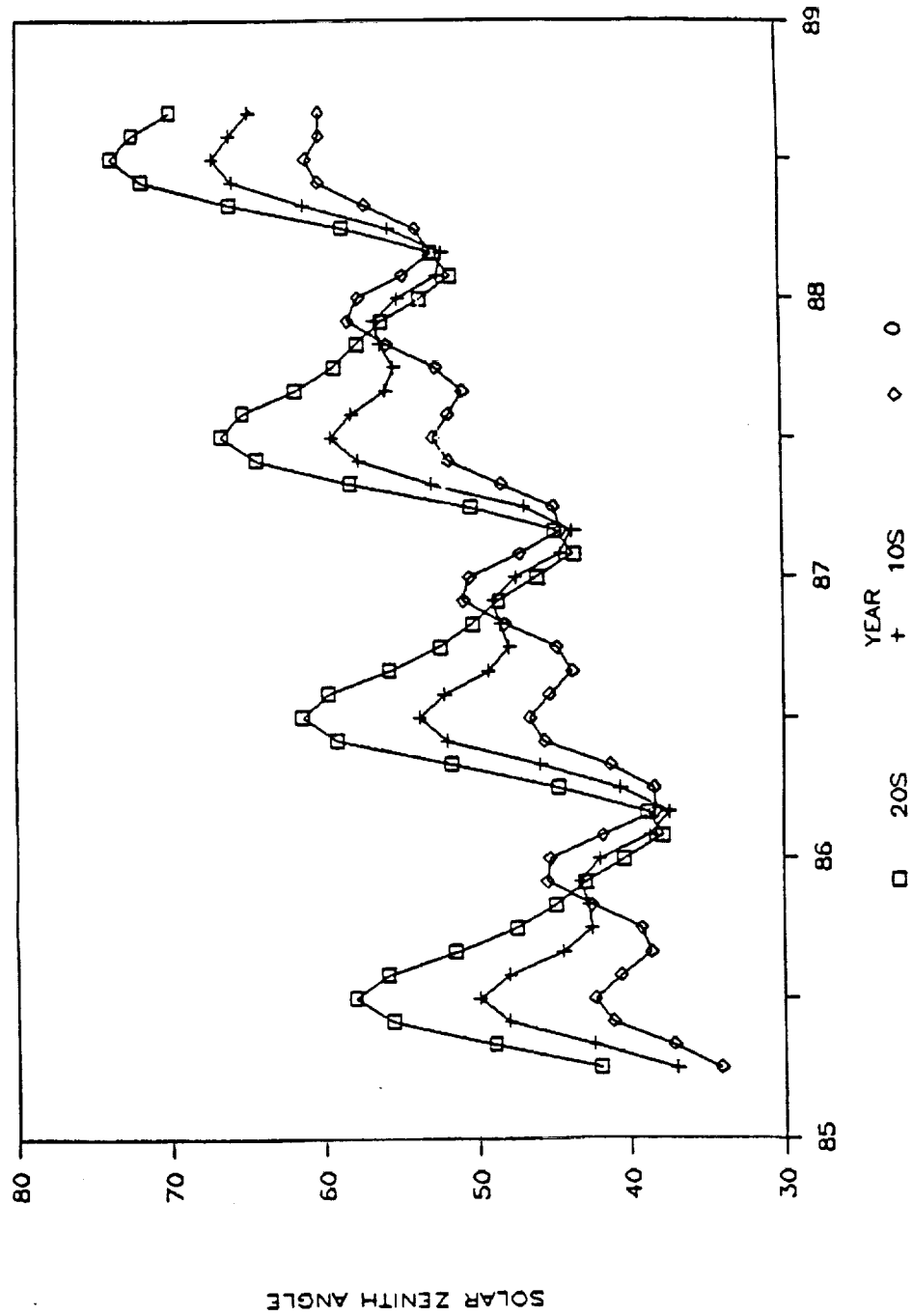
Figure 6. Results of linearity test applied to TOMS averaged, deseasonalized, adjusted N-value changes. (Indicates success in deriving ozone from adjusted mean N-value changes.)
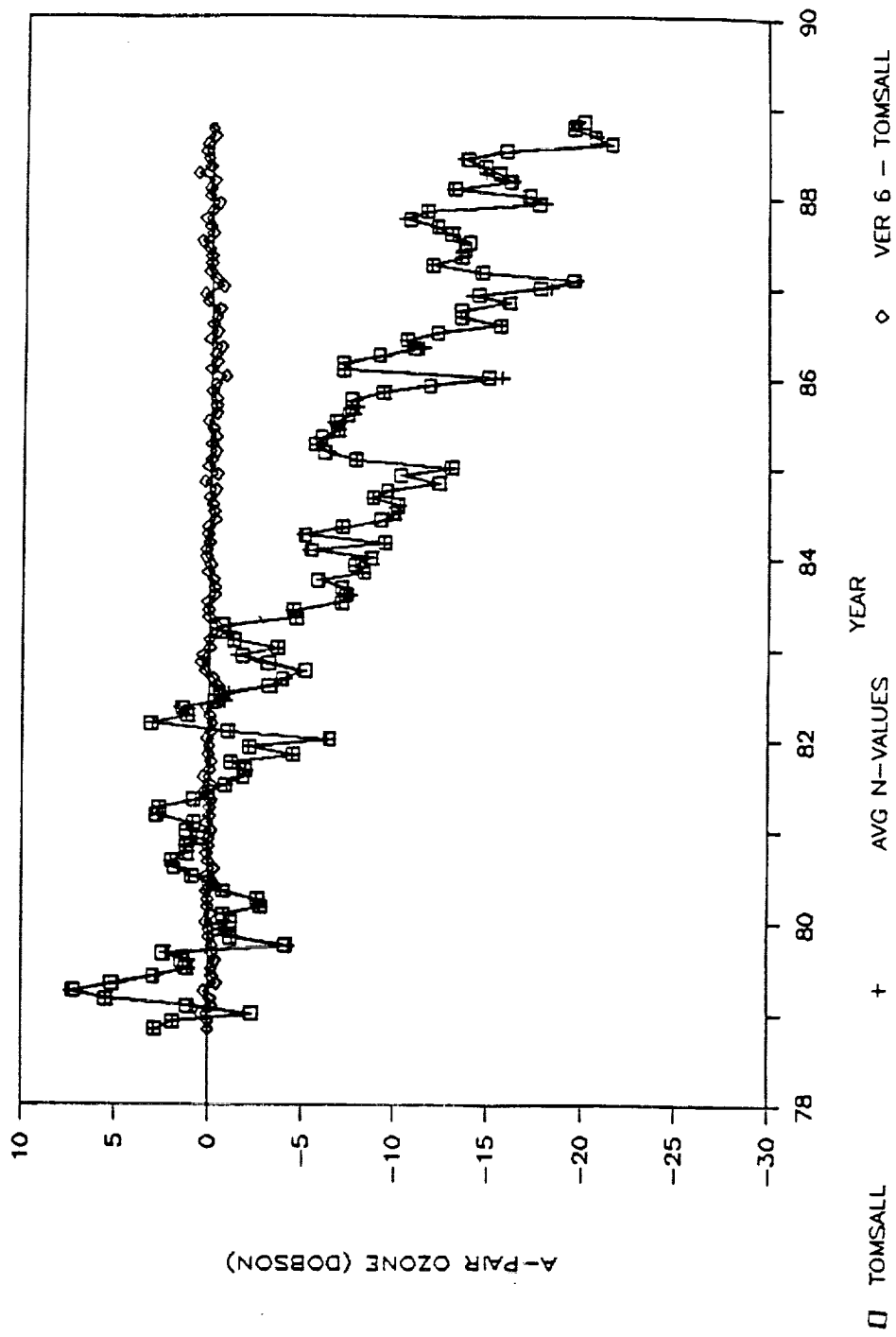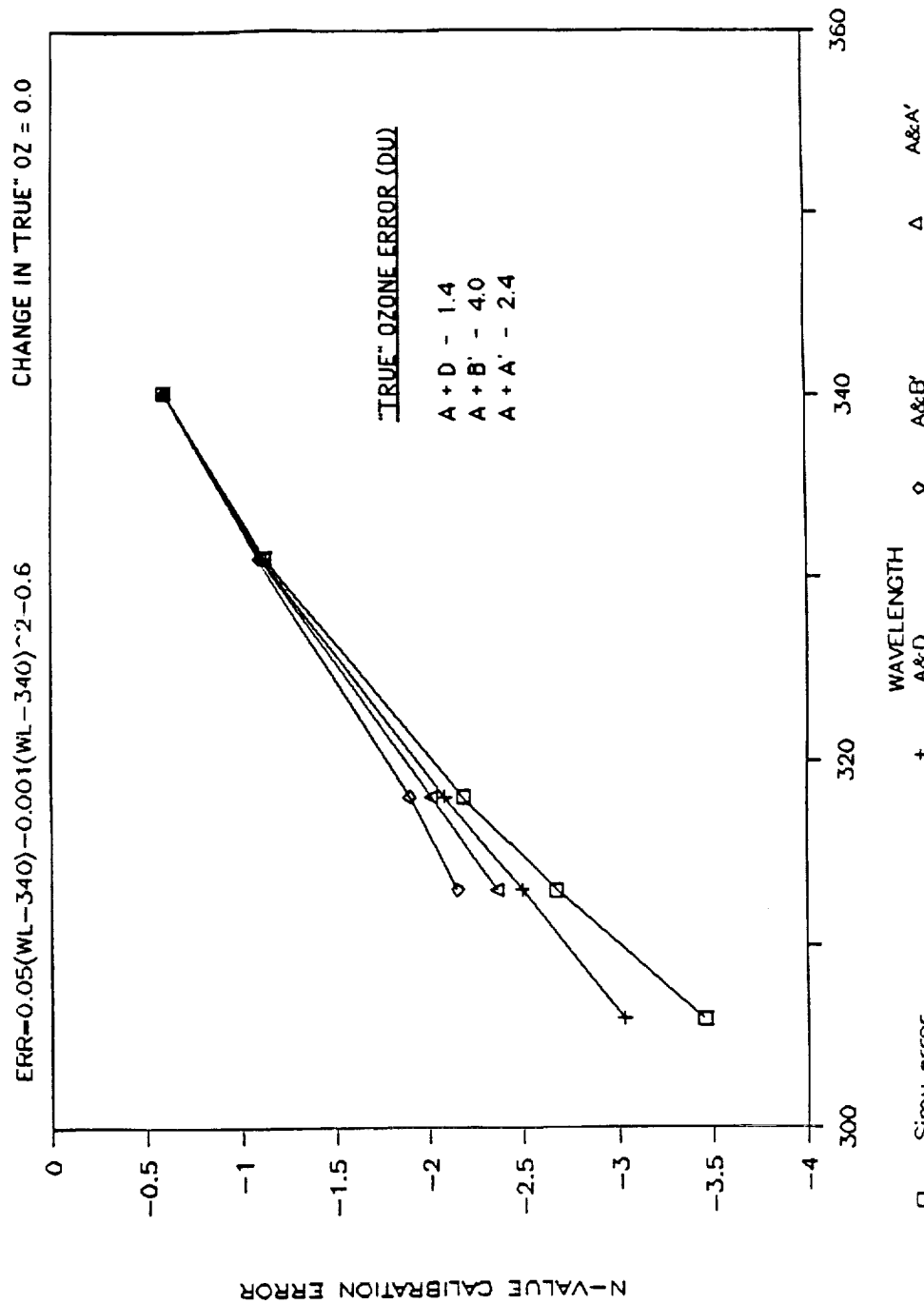
Figure 7. Results of linearity test applied to SBUV/2 averaged, deseasonalized, adjusted N-value changes. (Indicates limited success in deriving ozone from adjusted mean N-value changes.)
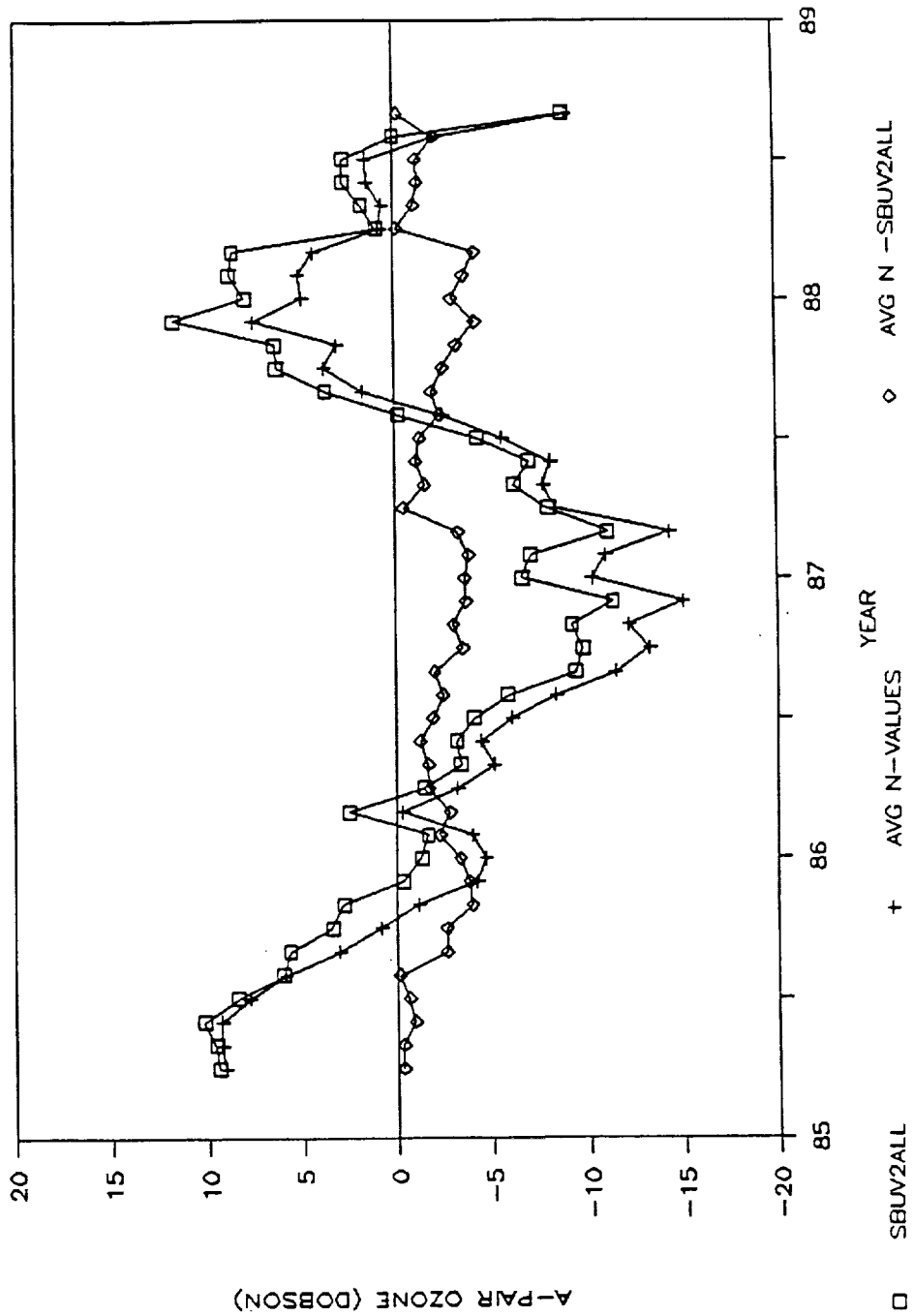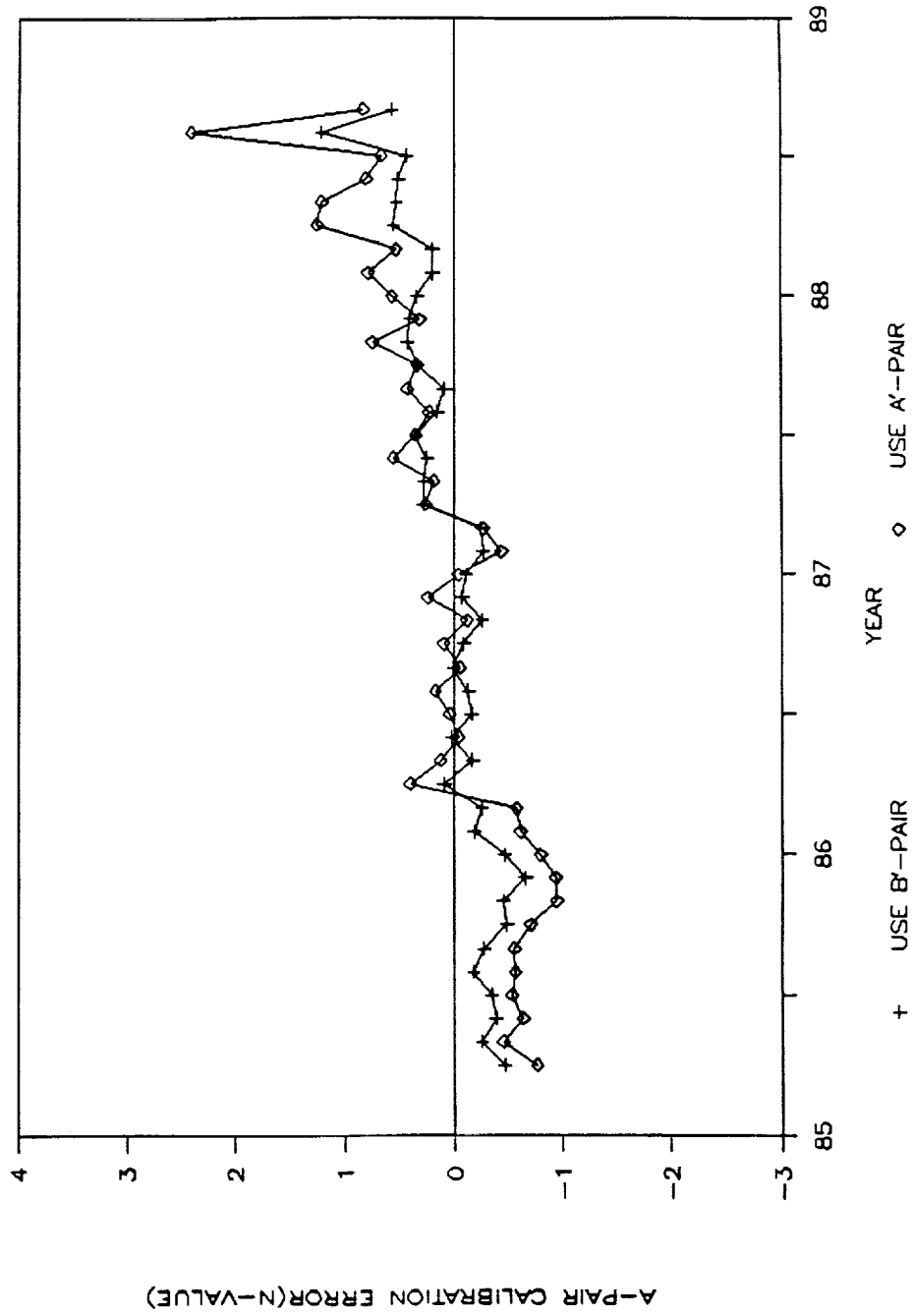
Figure 8. Results of pair justification technique applied to simulated N-value changes containing error that is linear in wavelength.

$$ERR = 0.05(WL-340)-0.6$$
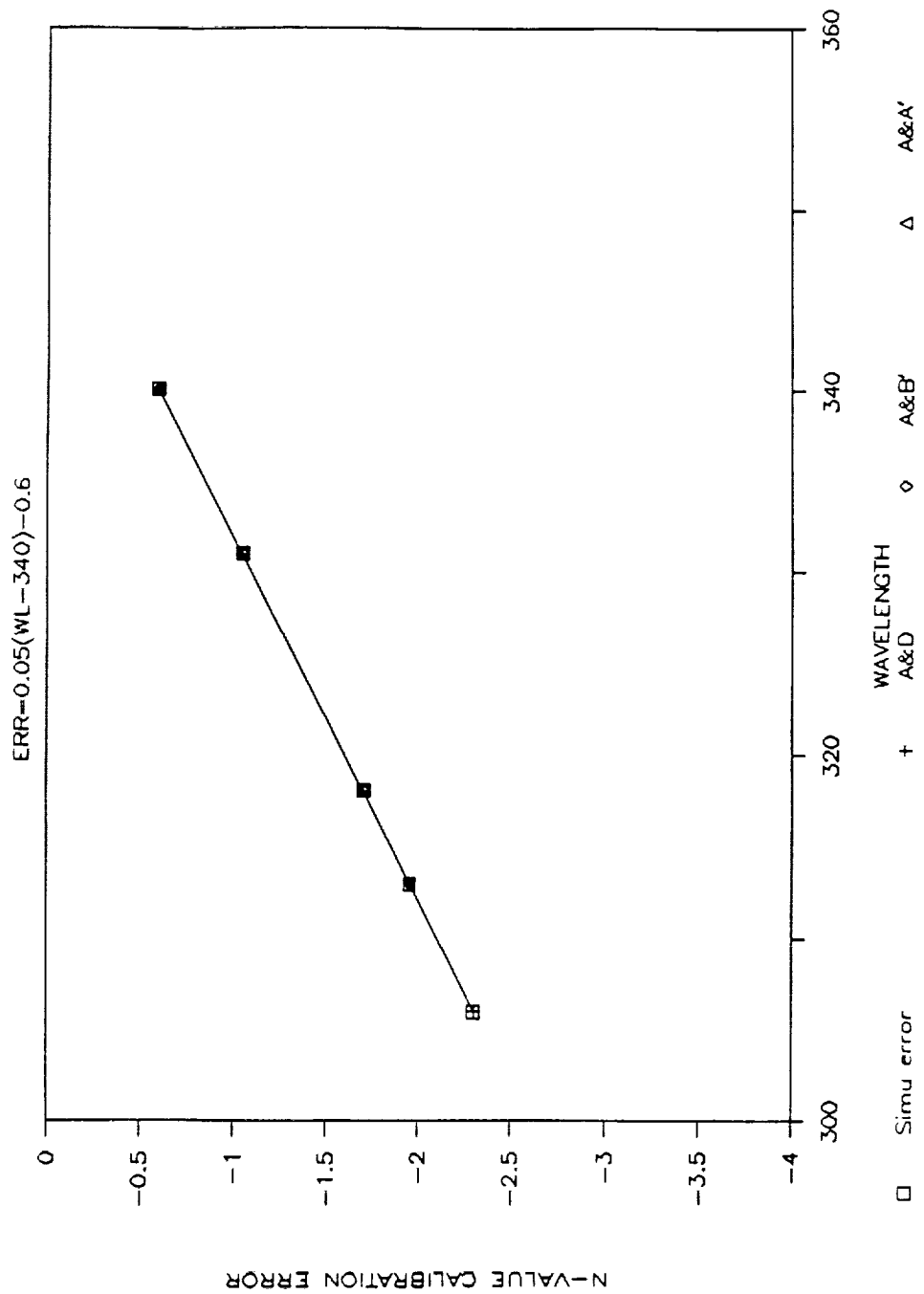
Figure 9. Results of pair justification technique applied to simulated N-value changes containing error that has second order wavelength dependence.

$$ERR = -0.05(WL-340) - 0.001(WL-340)^2 - 0.6$$

CHANGE IN "TRUE" OZ = 0.0

"TRUE" OZONE ERROR (DU)

A + D	- 1.4
A + B'	- 4.0
A + A'	- 2.4

N-VALUE CALIBRATION ERROR

WAVELENGTH

□ Simu error   + A&D   ◇ A&B'   △ A&A'

Figure 10. SBUV/2 A-pair calibration error derived using the pair justification technique

Figure 11. Error in SBUV/2 equatorial ozone derived using the pair justification technique

(LAT=0)

ERROR IN BEST OZ (D.U)

YEAR

□ USING A&B'   + USING A&A'
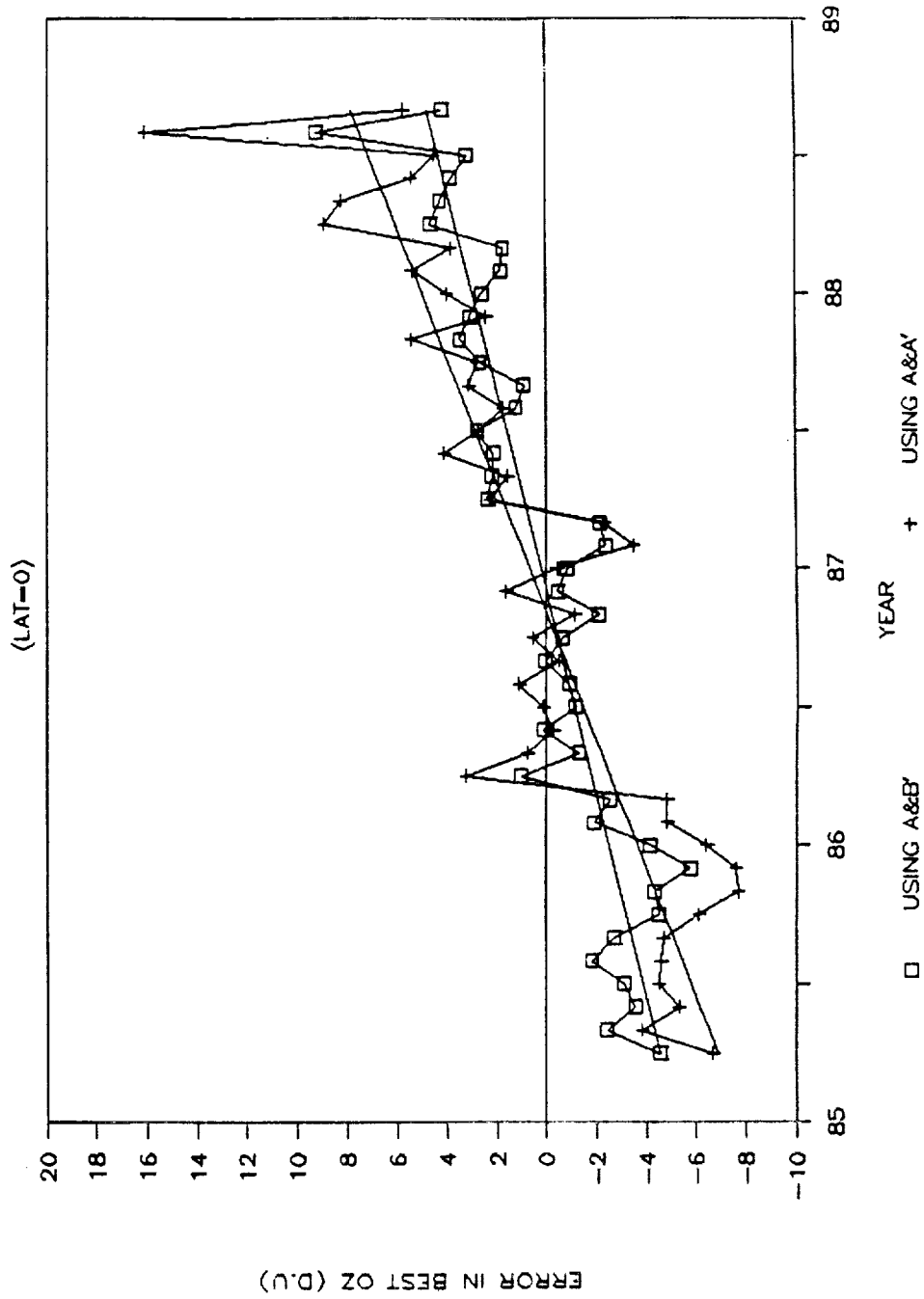
Attachment 10
Calibration of Long Term Satellite Ozone Data
Sets Using the Space Shuttle
E. Hilsenrath
NASA/GSFC