NOAA Technical Report NESDIS 23

The Use of TOMS Data in Evaluating and Improving the Total Ozone from TOVS Measurements

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National Environmental Satellite, Data, and Information Service

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Abstract

Total ozone from the Total Ozone Mapping Spectrometer (TOMS) has been regressed against brightness temperatures from the TIROS Operational Vertical Sounder (TOVS). The TOMS data provide a vast improvement over the amount of ozone data from the Dobson network currently used to compute the regression coefficients for the operational retrieval of total ozone from the infrared sounders on NOAA satellites. The TOMS data make it possible to derive regression coefficients for smaller latitude zones and, for the first time, in a straightforward fashion in the Southern Hemisphere. Improvements to be realized upon implementation of the new series of regression coefficients are detailed. As measured by the coefficients of variation, the average errors in the computed satellite ozone are reduced by more than 30 percent. Comparison with the TOMS total ozone shows that the operational TOVS total ozone exhibits a seasonally-dependent bias in the Northern Hemisphere and a nearly constant bias in the Tropics and Southern Hemisphere.

1. INTRODUCTION

The TIROS-N series of NOAA environmental satellites carries the TIROS Operational Vertical Sounder (TOVS) (Schwalb, 1978). These instruments sense the upwelling radiance from the earth and atmosphere on a nearly continuous basis. Two satellites are normally in operation, one crossing the equator at local times near 7 a.m. and 7 p.m. and the second crossing at local times near 3 a.m. and 3 p.m. The data acquired by these polar-orbiting satellites are used primarily to define the three-dimensional structure of atmospheric temperature and water vapor (Smith et al., 1979). In addition, it has been found that total ozone can be derived from these observations (Planet et al., 1984). The method employed is multiple linear regression where the total ozone derived from ground-based Dobson measurements is regressed against brightness temperatures in several of the TOVS channels. Planet et al. selected channels 3, 8, and 9 as predictors: the first sensing radiation near 15 μm from the lower stratosphere, the second sensing radiation in the atmospheric window at 12 μm, and the third channel sensing at 9.6 μm where atmospheric ozone radiates. Their studies were conducted with the data from TIROS-N, which ceased operation in May 1980. A continuation of those studies is reported here with the intent of developing improvements for the operational derivation of total ozone from the TOVS measurements.

In this study, the most significant departure from the earlier work is that the total ozone from the Total Ozone Mapping Spectrometer (TOMS) has been used in place of the Dobson values of total ozone. The TOMS instrument on Nimbus 7 has been described by Heath et al. (1975). The most significant impact of this change is that it provides a vast improvement in spatial coverage. Especially important is the opportunity to evaluate the north polar region and the Southern Hemisphere outside of the Tropics. In the previous study, no Dobson stations were available poleward of Barrow (71N) and Aspendale (38S). The entire southern hemisphere temperate zone was represented in that study by Aspendale. To overcome this deficiency of coverage in the Southern Hemisphere, the total ozone from the Dobson stations of the northern temperate zone were used with the limited Southern Hemisphere data of the same season in deriving the regression coefficients for that region. That approach, of course, forced the regression coefficients of the south temperate/polar zone to be nearly identical to the north temperate/polar zone coefficients for the same season.

An additional improvement to be expected when using the TOMS data is a reduction in variance of the observed ozone values used in determining the regression coefficients. With as many as 12 Dobson stations contributing observations to the data set from which the regression coefficients were derived in the previous study, relative biases among the various stations contribute to the errors in the predicted total ozone. However, with the TOMS observations, such biases are eliminated and real variance in the total ozone is added because of the global scope of the data sample. A single satellite observing globally provides a more extensive data base useful not only for deriving regression coefficients, but also for evaluating the quality of the derived ozone. Separate subsets of the matched TOVS/TOMS data are used for the derivation of the regression coefficients and for the evaluation of the quality of the derived ozone.

2. THE MERGED TOVS/TOMS DATA SET

The TOVS brightness temperatures, residing on archival tapes, have been combined with the total ozone derived from the measurements of the TOMS. The TOMS total ozone data (Heath et al., 1978) are daily average values archived in a 37x73 global array. Each grid point represents an area of 5° latitude by 5° longitude. Each TOVS measurement is assigned the total ozone value of the closest grid point of the TOMS array. Only daytime TOVS observations have been matched with the TOMS ozone measurements which are restricted to daytime by the measurement technique. One additional restriction was imposed on the data. The scan pattern of the TOVS instruments results in observations to either side of the sub-satellite track. Only those TOVS observations acquired in the two near-nadir angles of the six viewing angles were accepted because the data from the off-nadir angles are of reduced quality. The merged TOVS/TOMS data set used in this study extends from October 1979 to September 1982.

3. DETERMINATION OF SEASONAL/ZONAL PREDICTORS

The large amount of TOMS data permits the categorization of the data by geographic zones and time periods. Initially, a three-year sample of NOAA-6 data was grouped by latitude zones and season. Three-month periods beginning November 1979 and ending September 1982 were evaluated to determine the set(s) of predictors that produce the most accurate values of total ozone. Brightness temperatures from seven of the TOVs channels and the latitude of the observation were evaluated as predictors. From this set of eight predictors, those combinations of four predictors which best accounted for the variance in total ozone were tabulated for three Northern Hemisphere latitude zones: 0-30°, 30°-60°, and 60°-90°. The selection of predictors was based on computed values of R^2, a statistical measure of the amount of variance in the predictand explained by the predictors and is given by

$$R^2 = 1 - \frac{\Sigma_i^n(\Omega_i - \hat{\Omega}_i)^2}{\Sigma_i^n(\Omega_i - \bar{\Omega})^2} \qquad (1)$$

where Ω_i are the TOMS ozone observations, $\hat{\Omega}_i$ are the values of ozone from the regression model, $\bar{\Omega}$ is the mean of Ω_i and n is the number of observations.

An examination of the seasonal and latitudinal variations of the best predictors reveals the following. In the 0-30° and 30°-60° zones, distinct sets of predictors were found for each of the four seasons over the three-year period of the data. Neighboring seasons often were represented by the same sets of best predictors. It should be noted that, in most instances, nearly identical R^2 values were found for many combinations of predictors. No truly "best set" of predictors was usually found but rather a family of "best sets" with nearly identical values of R^2.

The situation for the 60°-90° zone is less clear. The same best sets of predictors were found only for the fall season of all three years. For the other three seasons the best predictors were more varied. For each of these seasons, common predictors were found for only two of the three years. These repeating annual patterns, although less predictable in the polar region, demonstrate that different sets of predictors for different seasons (or months, possibly) could be established from the historical data.

The TOMS data permitted, for the first time, an extensive evaluation of the effects of changing predictors with season and latitude zones in the Southern Hemisphere as well. These data make it possible to investigate the relationships between the total ozone in the Southern Hemisphere and the measurements by the NOAA spacecraft. The Dobson stations are so sparse in the Southern Hemisphere that coefficients for computing total ozone in the operational processing of NOAA data depend almost entirely on Northern Hemisphere coefficients adjusted for season. That circumstance forces the derived ozone in the Southern Hemisphere to be strongly influenced by the observed Northern Hemisphere ozone.

The R^2 values associated with various combinations of the TOVS channels were also computed for the Southern Hemisphere. The combinations of channels-seasons-latitude zones were restricted to the combinations employed in the Northern Hemisphere analysis. Three-month periods were treated together over three latitude zones between 90°S and 0°. The data used for this assessment were taken from a period beginning in November 1979 and extending to September 1982.

A tabulation of the five best sets of predictors was made for each three-month grouping of data for both hemispheres. The results from each 30° latitude zone throughout the nearly three years of NOAA-6 were examined and a single set of predictors selected as representative. The selected combinations are shown in Table 1 where $\bar{2}$, $\bar{4}$, and L refer to microwave channels 2, 4 and latitude, respectively. All other numbers refer to the channels of the HIRS instrument. Insufficient data were available for the Southern Hemisphere winter. Table 1 shows that different combinations of predictors were selected in the two hemispheres. The benefits of computing total ozone from separate predictors for each hemisphere are examined in the following sections.

TABLE 1. The optimum sets of predictors selected for NOAA-6

MONTHS/LAT	-90	-60	-30	0	30	60	90
11,12,1	2,9,10,L	8,9,$\bar{4}$,L	2,9,10,L	9,10,$\bar{4}$,L	3,8,9,$\bar{2}$	3,8,9,$\bar{4}$	
2,3,4	9,10,$\bar{4}$,L	2,8,9,L	2,9,10L	3,9,10,11	3,8,9,$\bar{2}$	10,$\bar{2}$,$\bar{4}$,L	
5,6,7	-	2,9,10,11	8,9,10,L	9,10,$\bar{2}$,L	9,10,$\bar{2}$,L	8,9,$\bar{4}$,L	
8,9,10	3,9,$\bar{4}$,L	2,8,9,L	8,9,10,L	8,9,10,$\bar{4}$	9,10,$\bar{4}$,L	9,10,$\bar{4}$,L	

4. CATEGORIZATION OF THE DATA

The question of selecting the most appropriate latitude zones was addressed by examining the latitudinal variation of the residual errors, $(\Omega_i - \hat{\Omega}_i)$, from the regression computations. The procedure was to compare the residuals obtained from regressions performed over each 10^o latitude zones. Typically, these latitudinal investigations showed that the zones 0-10°N and 10°N-20°N were similar. Zones 20°N-30°N began the transition region where stronger latitudinal variations become evident. Zones 30°N-40°N and 40°N-50°N show increasing residual errors with latitude. Maximum residual errors were usually reached in zones 40°N-50°N or 50°N-60°N with a subsequent decline as latitude increased beyond 60°N. On the basis of these results, four latitude zones were established in each hemisphere for all further computations. These are: 0 to 20, 20 to 40, 40 to 60, 60 to 90 plus the original zones selected for the operational processing, namely, -90 to -30, -30 to +30, and +30 to +90.

For each of the above latitude zones, calculations were performed to determine the reduction in the coefficients of variation when the improved predictors as specified in Table 1 were used on the dependent data sets of NOAA-6. The coefficient of variation is defined as

$$c.v. = 100\ \sigma/\bar{\Omega} \qquad (2)$$

where σ is the root mean square error of the residual ozone $(\Omega_i - \hat{\Omega}_i)$. Table 2 shows a comparison of these coefficients of variation for the 12 months of 1980 with the comparable values from the operational regression coefficients derived by Planet et al. (1984). Values are presented for each of the three operational latitude zones. The third column of each grouping shows the percent change. In nearly all cases, there is an improvement of between 10 percent and 40 percent. Averages at the bottom reveal consistent improvement over latitude. Several positive changes appear in the table. They are likely the result of improved predictors which are not optimum for that data set. Overall, the coefficients of variation are reduced by approximately 20 percent.

In sum, regression coefficients have been derived from improved sets of predictors. The values of the coefficients of variation associated with those predictors were shown to decrease by approximately 20 percent over the values used operationally. These demonstrated improvements are based on the three broad operational latitude zones. Further improvements may be obtained by utilizing the small latitudinal zones above. In addition, to get a more realistic assessment of the potential improvements in the total ozone computed from the TOVS measurements, one should apply the regression coefficients to independent data sets. This is the procedure followed in evaluating the coefficients used in the operational processing of the TOVS measurements. In that setting, regression coefficients derived from the data of a previous year are used to compute the total ozone derived operationally.

5. APPLICATION TO OPERATIONS

An operational situation was simulated so that the results of using the improved coefficients could be compared to the current operational results.

TABLE 2. Coefficients of variation derived from the operational regression coefficients (Oper.) and from the improved predictors (Imp.) for the dependent data of NOAA-6

MONTH/LAT.	30 to 90			-30 to 30			-90 to -30		
	Oper.	Imp.	Change	Oper.	Imp.	Change	Oper.	Imp.	Change
J '80	8.6	6.7	-22%	4.9	4.0	-18%	5.8	4.4	-24%
F	8.6	6.9	-20%	5.2	3.8	-27%	5.9	4.7	-20%
M	8.2	6.5	-21%	4.7	4.1	-13%	6.1	5.6	-8%
A	7.3	5.6	-23%	4.5	4.6	+2%	6.2	5.2	-16%
M	5.9	5.3	-10%	3.9	3.8	-3%	6.8	4.1	-40%
J	5.6	4.5	-20%	3.9	3.1	-21%	6.5	4.3	-34%
J	5.8	4.5	-22%	4.4	3.0	-30%	7.3	5.5	-25%
A	5.9	4.1	-30%	4.4	3.6	-18%	7.2	5.2	-28%
S	6.2	4.3	-30%	4.0	3.1	-22%	6.8	6.6	-3%
O	6.3	5.6	-11%	3.8	2.7	-29%	6.9	7.1	+4%
N	6.9	4.6	-33%	3.9	3.0	-23%	7.3	6.6	-10%
D	6.5	6.0	-8%	4.1	3.3	-20%	6.8	4.8	-29%
Avg. 1980			-20%			-18%			-19%

Calculations of total ozone were made for one month of each season of 1981 and 1982. The coefficients used in these calculations were derived from the corresponding months of 1980. Residual errors were derived for the data of January 1981 and 1982 based on Dobson operational coefficients of January 1980; residual errors based on the improved predictors were also derived. Similar computations were performed for the data of April and July of 1981 and 1982 and October of 1979 and 1981. Figure 1 shows the coefficients of variation of the residual ozone (Eq. 2) for the 11 latitude zones of the 1981 data sets. In the winter polar zones the data sets contain no data because only daytime observations have been included in this study. The TOVS data were restricted to daytime to match the TOMS observation period. Striking improvements are seen in several regions. In particular, the 20-40^{o} zone in the winter hemispheres (January and July), plotted at 30^{o}, show a marked reduction in the value of the TOMS-derived coefficients of variation relative to the Dobson-derived value. The partitioning of the tropical region into 20^{o} latitude zones permits the

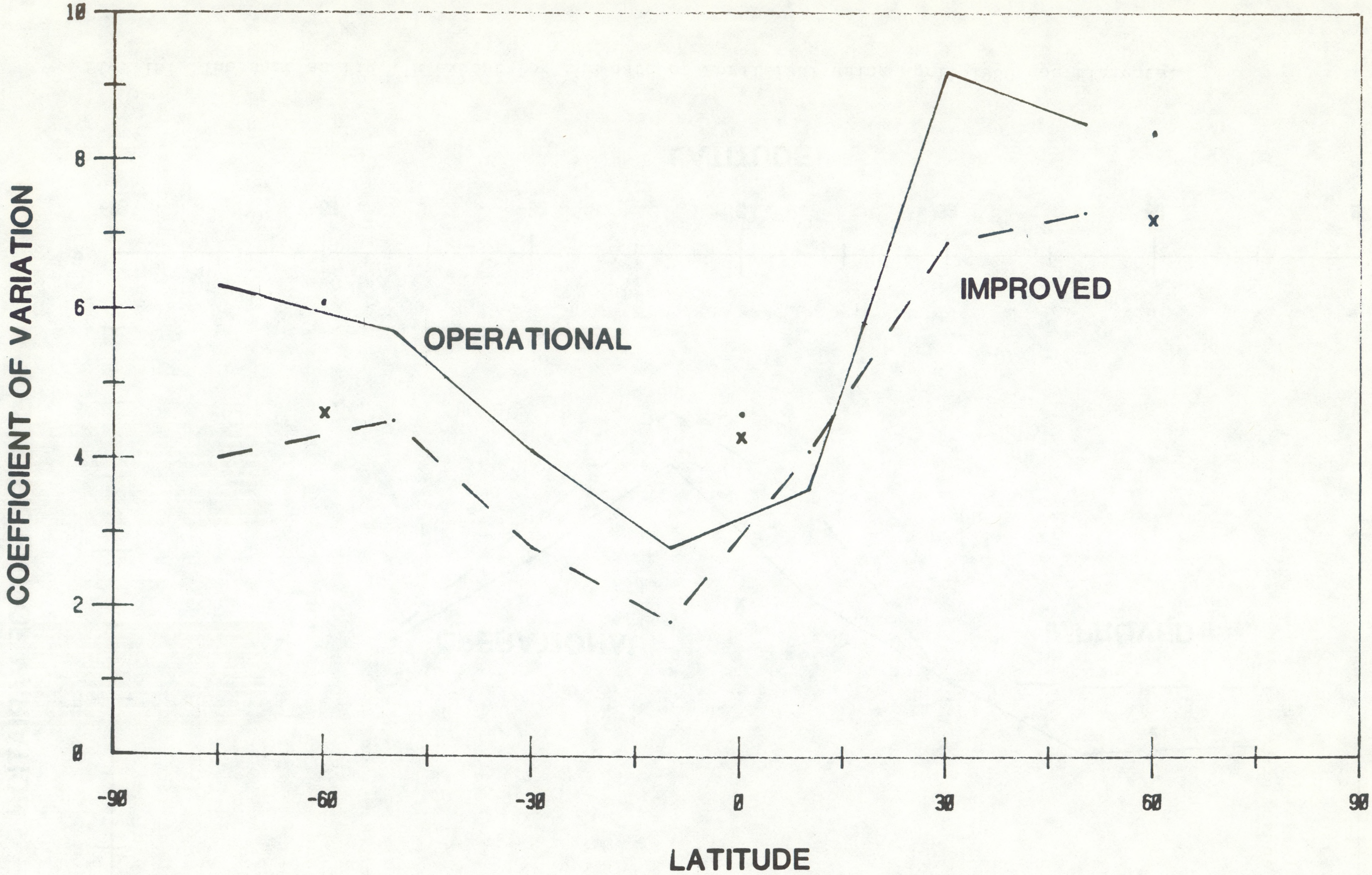

Fig. 1a. The coefficients of variation for various latitude zones from the data of January 1981 using regression coefficients derived from January 1980 data. The solid line represents the results from the operational Dobson-derived coefficients; the dashed line represents the results from the improved TOMS-derived coefficients. Dots and crosses show the values from the three operational latitude zones (90°S to 30°S, 30°S to 30°N, 30°N to 90°N) for the operational and improved coefficients, respectively.

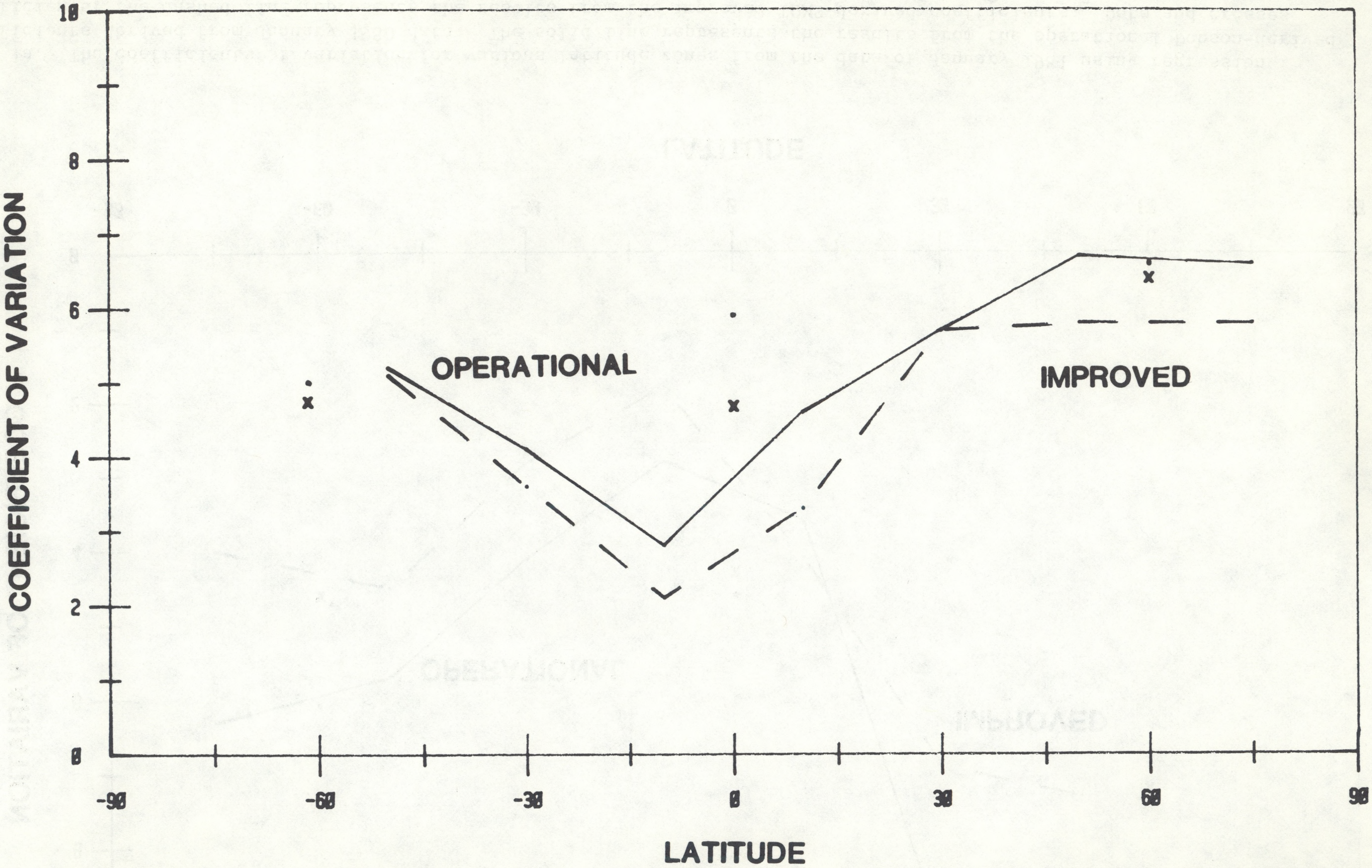

Fig. 1b. The same as Fig. 1a except for the data of April 1981 using April 1980 coefficients.

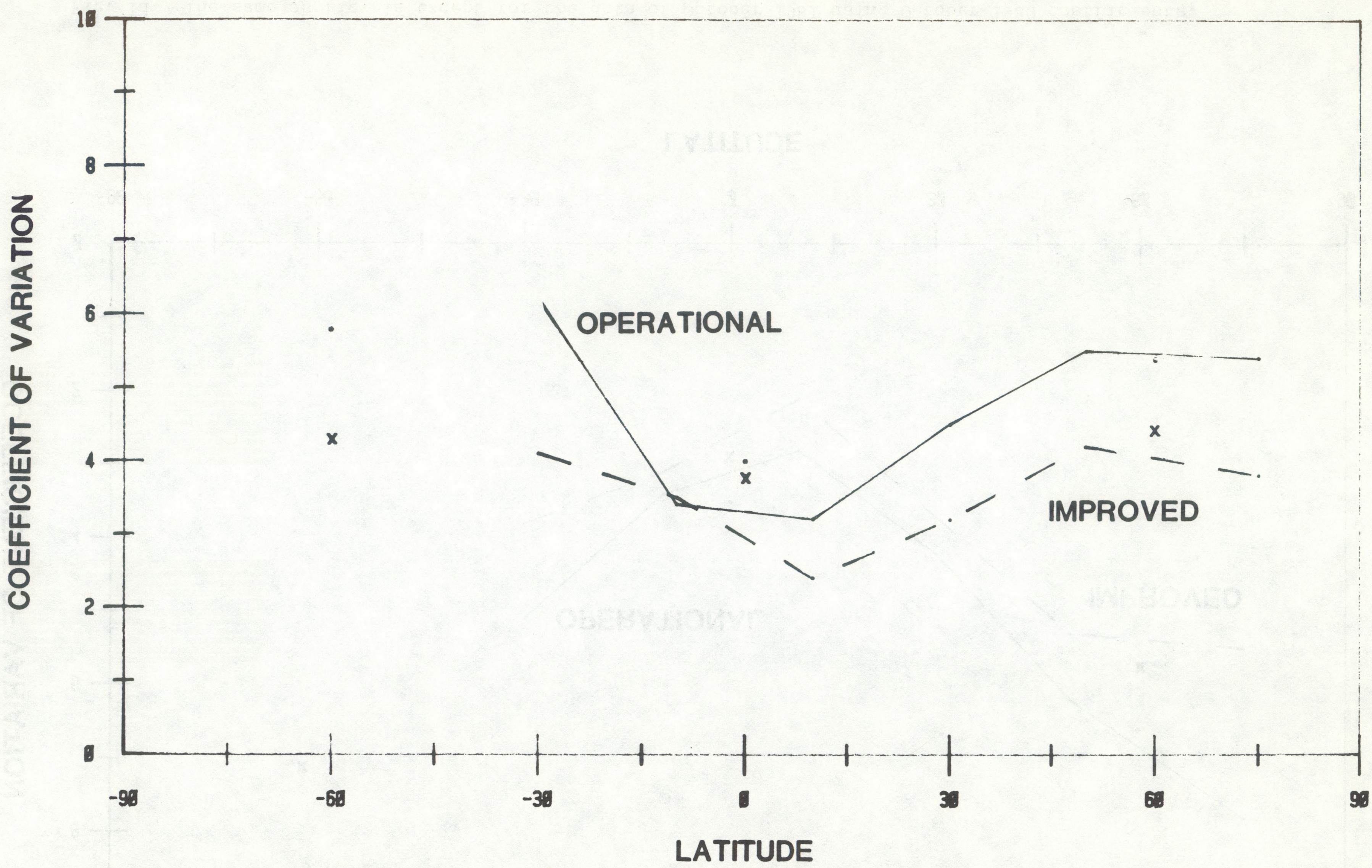

Fig. 1c. The same as Fig. 1a except for the data of July 1981 using July 1980 coefficients.

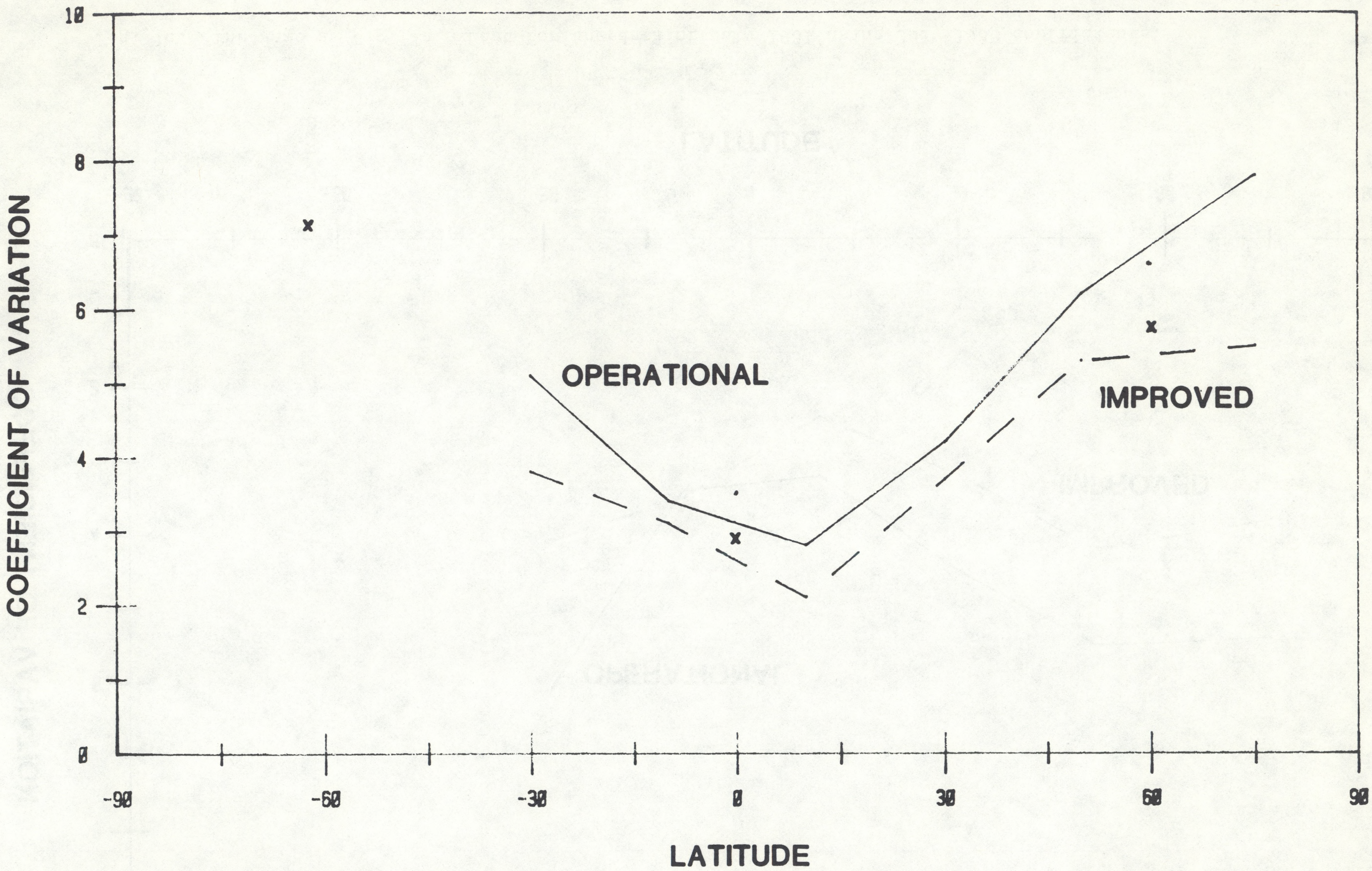

Fig. 1d. The same as Fig. 1a except for the data of October 1981 using October 1980 coefficients.

large differences between the data on either side of the equator in January and April to become apparent. The average reduction in the coefficients of variation is near one unit. This result is in essential agreement with Table 2, which shows a 20 percent reduction in the coefficient of variation within the dependent data set. In the Southern Hemisphere there is insufficient data in winter and spring, Figs. 1c and 1d, to assess the relative improvements south of the transition region, 20^{o}S-40^{o}S. Loss of data in the temperate and polar regions appears to be a consequence of the early morning time of observation by NOAA-6 coupled with the requirements in this study that all data be acquired during the sunlight portion of the orbit. A comparable study based on data from NOAA-7, which observes at midafternoon, would not be similarly restricted, thus providing more complete data sets in those regions.

It is interesting to compare the latitudinal distribution of the data in Fig. 1. During the Northern Hemisphere winter, January, a strong dependence of the coefficients of variation on latitude is seen in both hemispheres. In contrast, during the Southern Hemisphere winter, Fig. 1c, the latitudinal dependence is greatly reduced. Generally, Figs. 1a-d demonstrate the lack of symmetry in the residual errors between the two hemispheres. Also, they demonstrate the improvements in the residual errors which can be expected if regression coefficients are derived from a more optimum set of predictors. Although not shown, the data from January, April, and July of 1982 and October of 1979 support the conclusions drawn from Figs. 1a-d.

Table 3 summarizes the improvements resulting from substituting the improved predictors for the operational predictors on the independent data sets of 1981 and 1982. Shown in this table are the coefficients of variation for the three operational latitude zones. Values resulting from the use of the 1980 Dobson regression coefficients and the 1980 TOMS improved coefficients are tabulated along with the percentage change between the two values. The average value for each latitude zone appears at the bottom of the table. These values are in good agreement with the averages shown in Table 2, which contains the dependent data set.

The improvements obtained by combining better predictors and smaller latitudinal zones are shown in Table 4. For each monthly data set, coefficients of variation from the three operational zones were weighted by the sample size to derive a single global value. A similar computation was performed on the coefficients of variation from the improved coefficients over the eight narrow latitude zones. The percentage change in the global coefficient of variation is shown for each data set. Reductions in the global value range from 26 percent to 41 percent. The average improvement over the eight data sets is 32 percent. Reductions in the coefficients of variation of this magnitude can be reasonably expected upon implementation of a processing scheme incorporating smaller latitude zones and improved predictors.

Of significant interest is the reduction in the range of extreme errors (maximum residual error minus minimum residual error). Table 5 shows a tabulation of the changes in the range of extreme errors between the results using the operational predictors and the improved predictors. Although several entries in the table indicate that the operational predictors produced slightly better results, the majority of the entries show that the range of the extreme residuals is reduced with the improved predictors. The maximum reduction occurred

TABLE 3. Coefficients of variation derived from the use of 1980 operational regression coefficients (Oper.) and from the 1980 four improved predictors (Imp.) on independent data

	30 to 90			-30 to 30			-30 to -90		
	Oper.	Imp.	Change	Oper.	Imp.	Change	Oper.	Imp.	Change
Jan '81	8.4	7.2	-14%	4.6	4.3	-7%	6.2	4.6	-26%
Jan '82	9.3	8.1	-13%	5.6	4.7	-16%	5.9	4.6	-22%
Apr '81	6.6	6.4	-3%	5.9	4.7	-20%	5.0	4.7	-6%
Apr '82	7.3	6.0	-18%	6.2	5.4	-13%	4.3	3.9	-9%
Jul '81	5.4	4.9	-9%	4.0	3.9	-2%	5.8	4.3	-26%
Jul '82	5.8	4.4	-24%	3.8	2.9	-26%	7.9	5.5	-30%
Oct '79	7.5	6.4	-15%	3.8	3.3	-13%	7.9	6.4	-19%
Oct '81	7.8	5.5	-29%	3.5	2.9	-17%	9.6	7.2	-25%
Avg.			-16%			-14%			-20%

TABLE 4. Global weighted coefficients of variation based upon the three zones with operational predictors (Oper) and the eight narrow zones with the improved predictors (Imp.)

	Oper.	Imp.	Change
Jan '81	5.91	4.39	-26%
Jan '82	6.39	4.55	-29%
Apr '81	5.99	4.42	-26%
Apr '82	6.26	4.32	-31%
Jul '81	4.67	2.89	-38%
Jul '82	4.82	3.42	-29%
Oct '79	5.92	3.52	-41%
Oct '81	6.20	3.85	-38%

in the data of October 1979 in the 20°S-40°S zone where the range of the residuals decreased from 108 Dobson units to 50 Dobson units. Generally, the reductions are quite varied. The mean of the entries in the eight zones is 17 percent. The lack of data in the Southern Hemisphere winter polar regions is caused by the fact that NOAA-6 passes over those regions prior to sunrise.

TABLE 5. Percent change in range of extreme residuals resulting from using the improved predictors in place of operational predictors

Zone/Month	Jan		Apr		Jul		Oct	
	'81	'82	'81	'82	'81	'82	'81	'79
-90-60	-23	-34						
-60-40	-22	+2	-4	-7				
-40-20	-20	-32	-12	-15	-35	-8	-28	-54
-20 0	-35	-32	-2	-11	-29	-13	-9	-11
0 20	-16	-15	-29	-20	-20	-7	-20	+8
20 40	-9	-17	+7	-5	-17	-20	-2	-6
40 60	-24	-20	+3	-7	-15	-18	+6	-22
60 90			-4	-14	-23	-26	-22	-40
-90-30	-17	-16	-5	-10	-29	-15	-20	-22
-30+30	-10	-5	+3	-11	-17	-7	-14	-2
30 90	-25	-15	-5	-6	-12	-21	+3	-11

The paragraphs above have discussed the significant reductions in the residual errors made possible by using improved predictors and narrowed latitude zones. It is also important to ascertain if any bias is present in the TOVS total ozone. Because the Dobson stations from which the operational regression coefficients are derived are so sparse, it has not been possible previously to evaluate the TOVS ozone for bias except within limited geographical regions. Planet et al. (1984) showed monthly average differences between matched Dobson and TOVS total ozone amounts at selected locations. With the availability of the TOMS data, evaluation of the TOVS total ozone can be made for all regions of the globe. For this purpose the mean monthly TOMS total ozone has been computed for three latitude zones. The comparable TOVS total ozone has also been computed, using the operational regression coefficients. The values appear in Fig. 2 for the data of January 1980 through July 1982 within three latitude zones: the Northern Hemisphere (25N-55N), the Tropics (25S-25N), and the Southern Hemisphere (25S-55S).

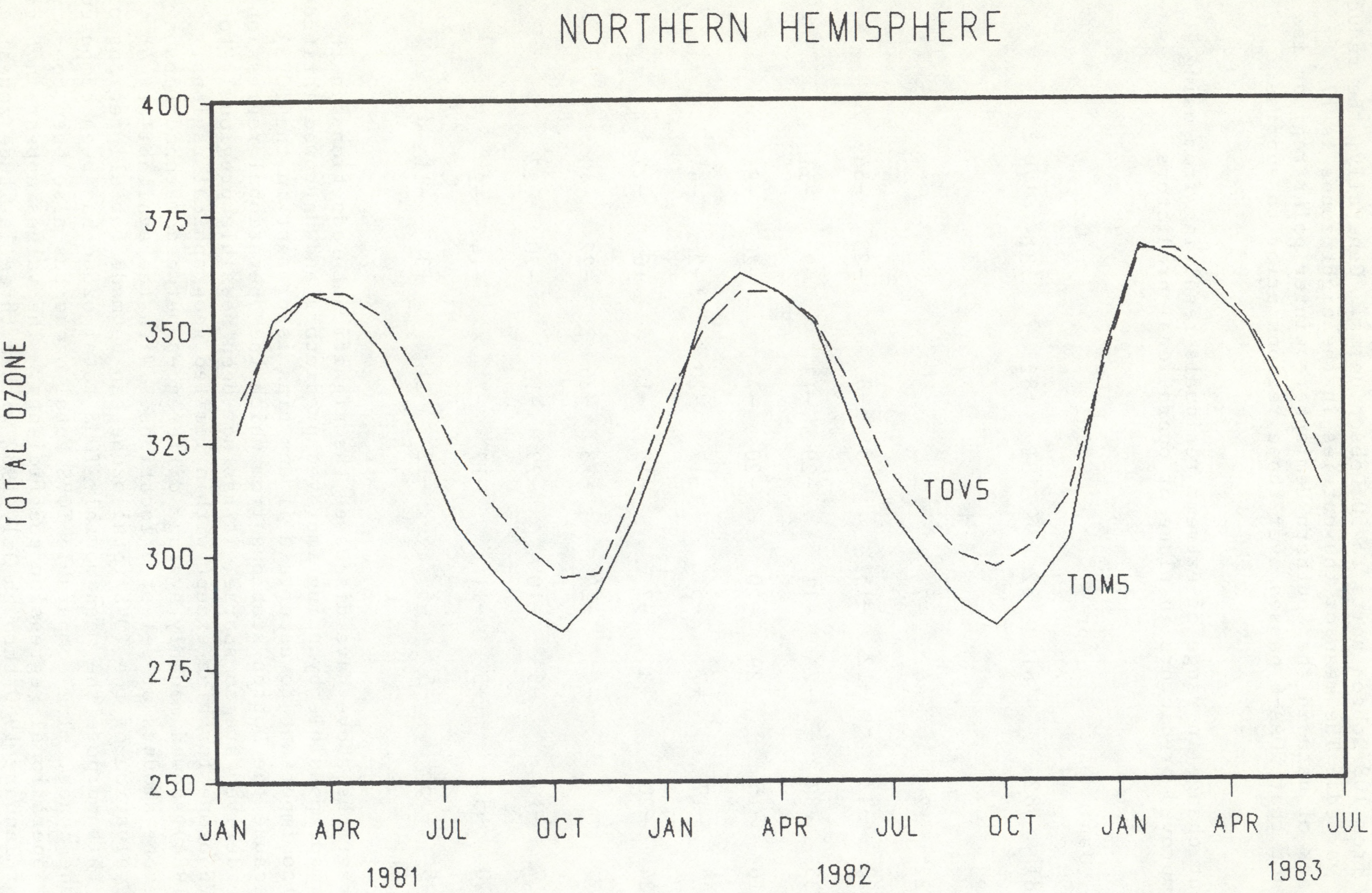

Fig. 2a. The annual variation of the NOAA 6 TOVS total ozone and TOMS total ozone for the 25N-55N zone.

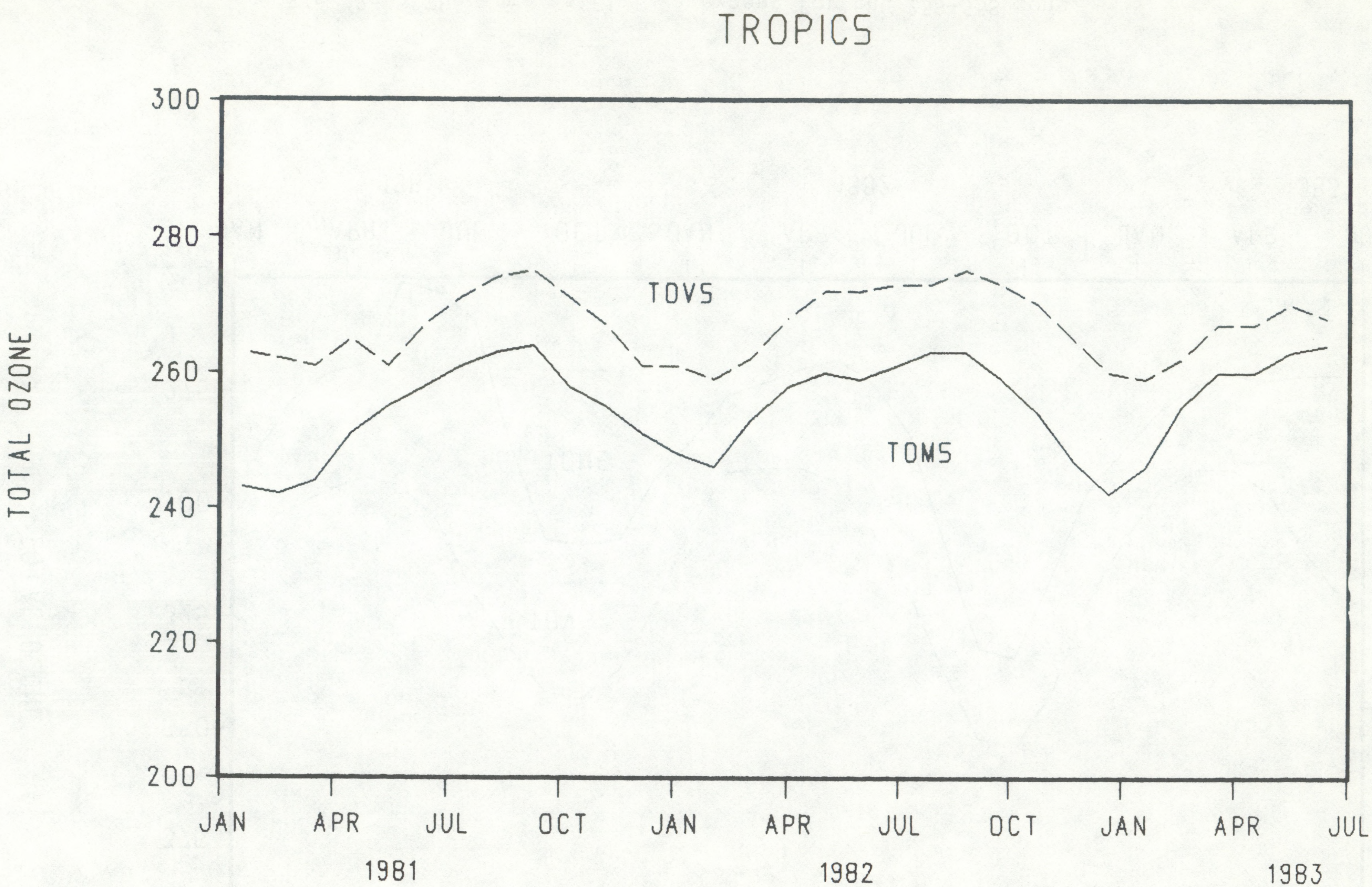

Fig. 2b. The same as Fig. 2a except for the 25S-25N zone.

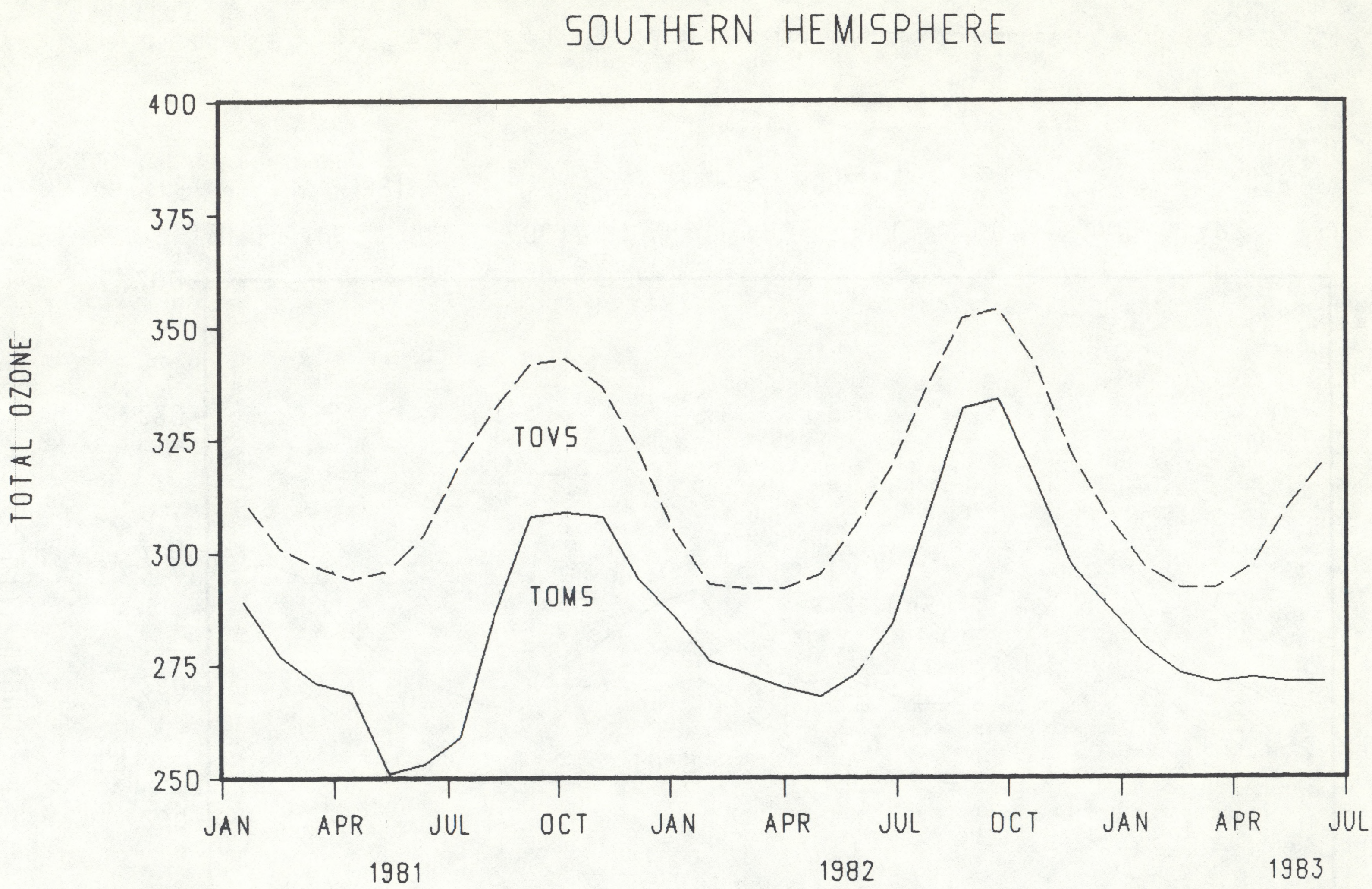

Fig. 2c. The same as Fig. 2a except for the 25S-55S zone.

Fig. 2 leads to an unexpected result, namely, the operational coefficients derived from the Northern Hemisphere Dobson measurements yield more consistently biased ozone values when applied to the Southern Hemisphere TOVS observations than they do when applied to Northern Hemisphere observations. Both in the Tropics, 25S-25N, and in the Southern Hemisphere, 25S-55S, a nearly constant bias exists between the TOMS ozone and the TOVS ozone. In fact, the annual bias is reasonably close to that found by Bhartia et al. (1984) between the TOMS and Dobson measurements, thereby inferring that the TOVS ozone is in good agreement with the Dobson measurements. Bhartia et al. report an approximate 6-7% bias with no seasonal or latitudinal dependencies. In Fig. 2 it is seen that in the Northern Hemisphere the bias is seasonally dependent. Only the summer and fall periods exhibit a bias close to that reported by Bhartia et al. The winter and spring periods show that the TOMS ozone and TOVS ozone are nearly equal. The TOVS ozone from the winter/spring seasons should be increased by about 20 Dobson units to match the bias shown in other regions. The large bias in the Southern Hemisphere winter is an artifact of the data sample in that period.

One would expect that the use of the Northern Hemisphere coefficients in the Southern Hemisphere would create bias errors in that region and not in the Northern Hemisphere as observed. However, this apparent contradiction probably occurs because the tendency to underestimate ozone maxima, a characteristic of the regression procedures, is offset in the Southern Hemisphere winter/spring by the use of regression coefficients derived from the ozone-rich Northern Hemisphere winter/spring. Thus, the consistent bias in the Southern Hemisphere, which is in excellent agreement with previous work, may be somewhat fortuitous. The inconsistent bias in the Northern Hemisphere is probably also related to the inability of the regression technique to retrieve high values of ozone in that region during the winter/spring periods of maximum ozone.

In summary, the TOVS data appear to have a relatively constant bias to the TOVS data in all regions except the Northern Hemisphere winter/spring where they appear to be about 20 Dobson units low. It is likely that this Northern Hemisphere inconsistency is related to the regression technique.

6. CONCLUSIONS AND RECOMMENDATIONS

The data presented in Fig. 1 and Tables 4 and 5 indicate the improvements in the determination of total ozone which may be realized by using the TOMS-derived coefficients in the operation. It is apparent that the combined use of the TOMS-derived improved predictors and the more refined latitude zones generally produce reductions in the coefficients of variation, particularly in the winter temperate zones. The differences between the two hemispheres indicate the need to treat each hemisphere independently. On the basis of Fig. 2, the satellite ozone derived from the Northern Hemisphere winter/spring is less accurate than that derived for other regions and seasons.

All results reported in this study deal with the data obtained from the NOAA-6 spacecraft. Even though the limited TIROS-N data seemed to support the findings of the NOAA-6 data concerning the best channels to be used as predictors of ozone, the data from NOAA-7, in an afternoon orbit similar to TIROS-N, should be examined. A comparison between the total ozone derived from NOAA-6 and NOAA-7 data should be undertaken prior to defining the most appropriate algorithms for the calculation of total ozone from the TOVS observations. The NOAA-7 data are not as subject to the restrictions imposed by the sunrise in the winter polar regions and therefore constitute a more complete data set.

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