On the relationship between Total Ozone Mapping Spectrometer (TOMS) ozone and hurricanes

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Received 14 May 2004; revised 6 December 2004; accepted 6 January 2005; published 22 March 2005.

[1] The Earth Probe (EP)/Total Ozone Mapping Spectrometer (TOMS) total ozone \( (O_3) \) data are employed in an investigation of the relationship between total column ozone and hurricanes. It is shown that variations of total ozone amounts are closely related to the formation, intensification, and movement of a hurricane. A high correlation between TOMS \( O_3 \) and upper level geopotential height is found within hurricanes. A regime-dependent high correlation between TOMS \( O_3 \) and vertically integrated potential vorticity fields is also found in a hurricane environment. Several regression models are developed for applying TOMS \( O_3 \) to hurricane initialization and data assimilation.


1. Introduction

[2] The day-to-day fluctuations of total ozone in a column of air (referred to as total ozone hereinafter) have long been observed. Such fluctuations were found to be mainly caused by daily variations of the synoptic environment through either advection, convection, or both [Dobson et al., 1929]. In the horizontal plane, northerly advection causes an increase in total ozone, while advection of air from the south results in a decrease. Vertically, downward motion associated with an upper tropospheric trough results in an increase in total ozone, whereas upward motion in association with an upper level ridge results in a decrease [Reed, 1950; Barsby and Diab, 1995]. Furthermore, regions of high total ozone content are associated with high mean integrated potential vorticity (MPV), low temperatures in the upper troposphere, a low tropopause, high temperatures in the lower stratosphere, and low pressures in both the upper troposphere and lower stratosphere [e.g., Normand, 1953; Ohring and Muench, 1960; Penn, 1964, 1965, 1966; Danielsen, 1968; Schubert and Munteanu, 1988; Orlainski et al., 1989; Mote et al., 1991; Riishojgaard and Källén, 1997].

[3] The proximity between ozone and various atmospheric variables has allowed scientists to study meteorological phenomena using total ozone data. Orsolini et al. [1998] identified storm tracks based on the total ozone fluctuations during the winter and spring using daily gridded Total Ozone Mapping Spectrometer (TOMS) \( O_3 \) data with \( 1^\circ \) latitude by \( 1.25^\circ \) longitude horizontal resolution. Davis et al. [1999] developed an algorithm for retrieving three-dimensional winds from TOMS \( O_3 \) fields under the balanced constraint. Olsen et al. [2000] diagnosed an intense cyclone in the midwestern United States between 9 and 10 November 1998 with a high-resolution mesoscale numerical model analysis and EP/TOMS \( O_3 \) observations. A close resemblance between the total ozone distribution and the geopotential height at 350-hPa isosurface was shown. A strong correlation between the total ozone and geopotential height, which was shown for synoptic scales by Stanford and Ziemke [1996], was also observed to exist on mesoscales. Waugh and Funatsu [2003] investigated the evolution and structure of stratospheric intrusions into the upper troposphere over the northern tropical Pacific using NCEP/NCAR reanalysis data, in situ ozone observations at Hilo, Hawaii, and level-3 TOMS \( O_3 \) data with a \( 1^\circ \) latitude by \( 1.25^\circ \) longitude resolution. Hudson et al. [2003] studied the characteristics of the profiles of total ozone in four different meteorological regimes: the tropical regime, the midlatitude regime, the polar regime, and the arctic regime. It was shown that each regime except for the arctic has a distinct range of ozone values which does not overlap with the values of other regimes. The agreement between the regime boundary positions determined by both potential vorticity and ozone is good. Jang et al. [2003] applied TOMS \( O_3 \) to cyclone prediction. In their study, a linear regression model was derived for simulating TOMS \( O_3 \) based on MPV and TOMS \( O_3 \) observations were assimilated into a mesoscale model using the linear regression model. A positive impact from assimilating TOMS \( O_3 \) measurements on the prediction of an east coast winter storm that occurred between 24 and 25 January 2000 was obtained, in terms of forecasting the cyclone track, intensity, and the cyclone-induced precipitation distribution and amount.

[4] Less attention has been paid to the application of ozone observations for hurricane studies. This is because most hurricanes occur in tropical and sub-tropical regions, where the correlation between ozone and MPV is generally weaker than in midlatitudes and where fewer direct observations are available for evaluating the accuracy of satellite observations such as TOMS \( O_3 \). Penn [1965] was probably the first study to attempt to identify the structure of hurricane from ozone observations. From U2 flight obser-
vations, an ozone-rich region was discovered within the center of Hurricane Ginny (1963), indicating a stratospheric intrusion into the hurricane’s eye. On the basis of the work of Reed [1950] and combining the Nimbus-7 TOMS $O_3$ with numerical model simulations, Rodgers et al. [1990] proposed that there must be an ozone-rich region at the center of a hurricane and that the tropopause within the core of hurricane is not simply as was previously proposed by Stear [1965] and Koteswaram [1967]. However, owing to the coarse resolution of ozone observations (1° latitude by 1.25° longitude) used in their study, an ozone-rich region within the center of a hurricane was unable to be clearly shown.

[5] This study explores the possibility of using TOMS ozone to improve hurricane prediction. Given the high correlation of TOMS ozone and vertical integrated mean potential vorticity (MPV) at synoptic scales, it is expected that the large-scale features of TOMS ozone observations, if incorporated into a hurricane model, will contribute greatly to an improved track prediction of tropical storms. This study seeks a proper way to incorporate TOMS ozone data into a numerical prediction model to better describe a hurricane’s environmental flow through its link to MPV.

[6] Additionally, owing to the lack of conventional observations over tropical oceans and difficulties in using cloud-contaminated satellite radiance observations, the initial vortices of tropical storms in large-scale analyses are often too weak. The four-dimensional variational (4D-Var) bogus data assimilation (BDA) scheme proposed by Zou and Xiao [2000] was found to be an effective procedure to use limited observational data to generate an initial bogus vortex which has several observed features (e.g., intensity and size) of the hurricane being initialized and whose state variables satisfy the forecast model equations.

[7] In the 4D-Var BDA scheme, a bogus sea level pressure (SLP) is first specified on the basis of TPC (Tropical Prediction Center) observed parameters [Park and Zou, 2004]. Four-dimensional variational data assimilation (4D-Var) is then implemented to generate fields of all model variables which contain the specified SLP and satisfy hurricane forecast model equations. Since TOMS total ozone provides useful tropopause information of a hurricane, the second goal of this study is to generate a more realistic initial vortex by adding this information into a 4D-Var hurricane initialization procedure. In other words, constraints on the tropopause height distributions based on TOMS ozone can be implemented in a hurricane initialization.

[8] The arrangement of this paper is as follows: The data set and the hurricane cases used in this study are described in section 2. In section 3, the breakdown of the correlation between TOMS $O_3$ and MPV is investigated in the presence of a hurricane. By dividing TOMS $O_3$ data points into two different regimes, a new algorithm that results in two regime regression models with smaller standard deviation errors and better correlations between TOMS $O_3$ and MPV is described. Horizontal structures and intensity changes of TOMS $O_3$ data within a hurricane are described in section 4. The correlation between TOMS $O_3$ and the geopotential height on the 340 K isotropic surface ($\Phi_{340K}$) within the central region of a hurricane is also presented in section 4. A conclusion and a discussion on the possible applications of TOMS $O_3$ in hurricane initialization using the empirical models developed in this study are included in section 5.

2. Data Sets and Hurricane Cases

[9] In this paper, meteorological variables are obtained from the National Centers for Environmental Prediction (NCEP) reanalysis data set. The original analysis fields at mandatory pressures levels and with a horizontal resolution of 2.5° × 2.5° are interpolated to model grid points with a horizontal resolution of 45 km. Since the dynamic tropopause lies around 100 hPa, the model’s top pressure level is set to 50 hPa. The MPV is calculated by

$$MPV = \frac{1}{\Delta P} \int_{P_1}^{P_2} \frac{\eta}{\rho} \cdot \nabla \mathbf{d},$$

where ρ is the density of the atmosphere, $\eta = f \mathbf{k} + \nabla \times V$ is the 3-D absolute vorticity, $\theta$ is the potential temperature, $P$ is the pressure, $P_1 = 400$ hPa, $P_2 = 50$ hPa, and $\Delta P = P_1 - P_2$. The unit of MPV is PVU (1 PVU = 10^-6 m^2 K kg^-1 s^-1).

[10] Total ozone is measured by the EP/TOMS spectrometer. It uses the solar backscatter of six ultraviolet wavelengths from 308.60 nm to 360.40 nm to separate the effect of ozone absorption from the effects of cloud and ground reflection and scattering, thereby determining the total ozone amount. EP/TOMS measures total ozone at local noon with 90% daily global coverage. The highest possible nadir instantaneous field of view (IFOV) is approximately 40 km. For EP/TOMS $O_3$ observations, the estimated absolute error is ±3%, and the random error is ±2%. Detailed information of EP/TOMS data set is given by McPeters et al. [1998]. The unit of the total ozone used in this study is DU (Dobson unit), where 1000 DU = 1 atm cm under standard temperature and pressure.

[11] The raw non-gridded level-2 TOMS $O_3$ data set is used in most of the calculations conducted in this study. Only in the calculation of radial profiles of TOMS $O_3$ and the study of the correlation between TOMS $O_3$ and $\Phi_{340K}$ within hurricanes is the gridded TOMS $O_3$ used. The gridded TOMS $O_3$ data has a horizontal resolution of 45 km and is obtained by a Cressman analysis method with an influence radius of 500 km.

[12] Eleven hurricanes that occurred in the North Atlantic Ocean in August and September from 1996 to 2003 and one typhoon that formed in the western Pacific Ocean in September 2001 are chosen for this study. These are hurricanes with an intensity of category 2 or greater according to the Saffir-Simpson scale. The names, time periods, domains, and categories of these storms are provided in Table 1 and their tracks are shown in Figure 1. Hurricane Erin (2001) is chosen as a representative case to show many detailed variations of TOMS ozone due to an almost continuous full coverage of TOMS $O_3$ of this hurricane, except on 9 September 2001. A brief synoptic overview of this hurricane is given below.

[13] Erin’s lifecycle began off western Africa as a tropical wave on 30 August 2001. This tropical wave strengthened into a tropical storm by 0600 UTC 2 September. However, it did not rapidly evolve into a hurricane due to the presence of southwesterly wind shear. In fact, by 5 September the tropical cyclone degenerated into a depression. At 1800 UTC
Table 1. Names, Time Periods, Horizontal Domains, and Saffir-Simpson Scale Categories of the 11 Hurricanes and One Typhoon Included in This Study

<table>
<thead>
<tr>
<th>NAME</th>
<th>Data Period</th>
<th>Domain</th>
<th>Scale</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isabel</td>
<td>06 Sept. to 19 Sept. 2003</td>
<td>10°N–60°N, 85°W–30°W</td>
<td>5</td>
</tr>
<tr>
<td>Fabian</td>
<td>27 Aug. to 08 Sept. 2003</td>
<td>10°N–60°N, 75°W–20°W</td>
<td>4</td>
</tr>
<tr>
<td>Isidore</td>
<td>14 Sept. to 27 Sept. 2002</td>
<td>7°N–53°N, 68°W–12°W</td>
<td>3</td>
</tr>
<tr>
<td>Nari</td>
<td>06 Sept. to 21 Sept. 2001</td>
<td>6°N–50°N, 96°E–146°E</td>
<td>3</td>
</tr>
<tr>
<td>Felix</td>
<td>07 Sept. to 19 Sept. 2001</td>
<td>5°N–52°N, 105°W–45°W</td>
<td>3</td>
</tr>
</tbody>
</table>

7 September, Erin regained its tropical storm intensity, and strengthened into a hurricane by 2100 UTC 8 September. Its maximum wind speed by that time increased to 65 kt and its minimum SLP fell to 994 hPa around 0000 UTC 10 September. The observed “best track” of Hurricane Erin is included in Figure 1. It reached its peak intensity of 105 kt maximum sustained winds and a minimum SLP of 969 hPa around 0000 UTC 10 September, Erin regained its tropical storm intensity, and then began to weaken as it moved over cold waters and over the ensuing days, due in part to slightly warmer than normal waters over the western sub-tropical Atlantic. By 0000 UTC 15 September, Erin had weakened into a tropical storm and transitioned into an extra-tropical system 6 hours later. It merged with a high-latitude cyclonic low over eastern Greenland on 17 September 2001. A detailed report on Erin is given by R. J. Pasch and D. P. Brown (Tropical cyclone report hurricane Erin, available at http://www.nhc.noaa.gov/2001erin.html).

3. Regime-Dependent Linear Regression Models for Simulating TOMS $O_3$ Based on Large-Scale MPV in the Presence of a Hurricane

As a promising tracer in the upper atmosphere on the synoptical timescale, the daily TOMS $O_3$ observations may be beneficial for monitoring the mutual adjustment between the tropical cyclone and its upper tropospheric environment [Rodgers et al., 1990; Stout and Rodgers, 1992]. First, the relationships between TOMS $O_3$ and MPV during Hurricane Erin will be examined. Hurricane Erin transversed the domain bounded by 14.11°N–59.35°N and 91.68°W–35.82°W. The time span for TOMS $O_3$ observations to cover this domain is about 5 hours each day, centered around 1500 UTC. Therefore NCEP reanalysis data at 1500 UTC is used for calculating values of MPV, SLP, and $\Phi_{500\text{hPa}}$ on analysis grid points, which are then interpolated onto TOMS $O_3$ observation points. The correlation between TOMS $O_3$ and MPV in the given domain covering the period from 4 to 17 September 2001 is 0.818. This correlation compares well to correlation values of 0.81 and 0.82 obtained for a winter storm case in the middle latitudes, with horizontal resolutions for MPV of 30 km and 90 km, respectively [Jang et al., 2003]. On the basis of this high correlation, a linear regression model is derived from a least squares fit based on all data between 4 and 17 September 2001 within the domain,

$$O_3 = 6.084 \cdot \text{MPV} + 258.74. \quad (1)$$

Figure 1. “Best track” of selected storms. The locations at 0300 UTC and 1500 UTC are given. The data are downloaded from http://weather.unisys.com/hurricane/.

Figure 2. Daily variation of the correlation between TOMS $O_3$ and MPV at 1500 UTC for Hurricane Erin between 4 and 17 September 2001. TOMS $O_3$ level-2 raw data are used in this analysis.
The standard error of the MPV-simulated total ozone estimate (STDE) is 10.84 DU, which is comparable to the TOMS observational error. About 14.5% data points have a regression error greater than 1.4 STDE. 

[15] The correlation between TOMS $O_3$ and MPV experiences a large daily variation. For example, the correlation decreases sharply to less than 0.6 (see Figure 2) when Hurricane Erin intensified on 9–10 September 2001. Similar results are obtained with other hurricanes listed in Table 1.

[16] Realizing the strong degradation of correlation between $O_3$ and MPV when a strong hurricane is present, it is probably not appropriate to use (1) for TOMS ozone data assimilation within a hurricane environment. Instead, we propose to use regime-dependent linear regression models for hurricane data assimilation using TOMS $O_3$ data.

[17] A commonly used approach for improving the quality of a regression model which involves removing some “bad points” or “outliers,” i.e., points at which fitting errors are greater than a given threshold value, is utilized. Hereinafter, the outliers are to be referred to as “wild points.” Figure 3 shows TOMS $O_3$ and MPV distributions at 1500 UTC 9 September 2001 (Figure 3a), and the accepted and rejected sites of TOMS $O_3$ observations at which the difference between observed and simulated TOMS $O_3$ using the linear regression model (1) is 1.3 times larger than STDE (Figures 3b and 3c). The wild points are concentrated mainly in two types of regions. The first is the ozone-poor region where TOMS $O_3$ observations are slightly lower than climatology, and the other is the ozone-rich region in the middle to higher latitudes where TOMS $O_3$ values are greater than 293 DU. The flow patterns of TOMS $O_3$ and MPV are in close agreement in regions where TOMS $O_3$ is greater than 293 DU in the middle to higher latitudes. Specifically, there are two regions where TOMS $O_3$ are greater than 293 DU. One is located at the northwest corner of the domain; the other is in the eastern part of the domain. These high total ozone regions are characterized by either large stratospheric intrusion or...
northerly advection. Therefore TOMS $O_3$ data at these points contain useful meteorological information and should not be removed from data assimilation.

[18] On the basis of the above observations, a new procedure separating TOMS $O_3$ into two different regimes is devised. Each regime has its own linear regression model. In regions where the hurricane’s influence is weak, the close relation between the TOMS $O_3$ and MPV persists, while in regions that are strongly influenced by hurricane-induced deep convection, total ozone decreases greatly, and therefore a new relationship between the two quantities is necessary in order to use TOMS $O_3$ data more effectively. A detailed procedure for defining two such data regimes is described below, along with the two regime-dependent linear regression models.

[19] 1. To determine the first regime, perform the following. (1) Choose the points at which TOMS $O_3$ is greater than 293 DU, and denote these points as set $D_{293DU}$. Carry out a least square fit between observed and simulated $O_3$ in order to obtain the first linear regression model, and denote its STDE as $\sigma_1$. Set $k = 1$. (2) Remove those points in $D_{293DU}$ where the fitting error of the $k$th linear regression model is greater than $1.4\sigma_k$. Repeat the least squares fit to obtain the next linear regression model and denote its STDE as $\sigma_{k+1}$. (3) Repeat step 2 for $k = 2, 3$. (4) Denote the maximum fitting error of the third linear regression model as $\sigma_{\text{max}}$. All points in which the fitting error to the third linear regression model lies between $[-\sigma_{\text{max}} - 0.2, \sigma_{\text{max}} + 5]$ are taken as points in the first regime $S_I$.

[20] 2. Once regime $S_I$ is chosen, a least squares fit of all points in $S_I$ can be conducted to derive the first regression model. For Hurricane Erin, the following model in regime $S_I$ is determined:

$$O_3 = 6.429 \cdot \text{MPV} + 261.896.$$  \hspace{1cm} (2)

[21] 3. For the remaining points not in $S_I$, first obtain the least square linear regression model with its standard error of the estimate denoted by $\sigma'$. All points not in $S_I$ and whose regression error is less than $1.4\sigma'$ are placed into the second regime $S_{II}$. A least square fit of all points in $S_{II}$ will give the second regression model. For Hurricane Erin, the linear regression model in the second regime is obtained as follows:

$$O_3 = 6.005 \cdot \text{MPV} + 245.850.$$  \hspace{1cm} (3)

[22] All points which do not belong to either $S_I$ or $S_{II}$ are taken as wild points and are placed into the third group of points, $S_{III}$. It should be pointed out that the numbers we choose in developing the regime-dependent regression models may be altered for other hurricanes.

[23] Comparing two regime-dependent models (models 2 and 3) and the regression model (model 1) obtained without regime separation, it is found that both the slope and intercept of the regression model in $S_I$ ($S_{II}$) are greater (smaller) than those of the regime-independent model. Figure 4 depicts the scatter diagram of TOMS $O_3$ and MPV for Hurricane Erin during the period from 4 to 17 September 2001. The black dots are points in $S_I$, and the blue line represents the linear regression model for regime $S_I$. The red triangles are points in $S_{II}$ and the corresponding linear regression model (model 3) is represented by the yellow line. The green pluses indicate wild points.

**Figure 4.** Scatter diagram of TOMS $O_3$ versus MPV for Hurricane Erin, including all data from 4 to 17 September 2001. The black dots are points in which the regression error to the linear regression model (1) lies between $[-11.294, 16.095]$. The blue line is the corresponding regression line. The red triangles are points in which the regression error lies between $[-14.82, 14.82]$. The yellow line is the corresponding regression line. Finally, the green pluses indicate wild points.

[24] The day-to-day variations of correlation and STDE of the regression models (models 2)–(model 3) are compared with those of model (1) for Hurricane Erin in Figure 6a. The results in Figure 6b, in which the regression parameters are obtained from the data 1 day preceding to the date of calculation, are intended for finding the sensitivity of regime-dependent regression models to data amount and also represents a case in which TOMS $O_3$ data are to be used for hurricane prediction. No significant differences are observed between Figures 5a and 5b for regime determination (i.e., the locations and numbers of regimes $S_I$, $S_{II}$, and $S_{III}$), and between Figures 6a and 6b for correlation and standard error. In both cases, the separation of regime $S_{II}$ from regime $S_I$ not only improves the correlations between the TOMS $O_3$ and the MPV, but also significantly reduces STDEs of corresponding regression models throughout the entire period considered. The daily variations of the total numbers of TOMS $O_3$ observational sites in three different regimes from 4 to 17 September for Hurricane Erin are given in Figure 7. Only a very small portion of data points is...
removed daily. Moreover, for the full period from 4 to 17 September, the STDEs for the linear regression models (2) and (3) are 5.950 and 5.454 DU, respectively, which are only about half of the STDEs of model (1). Moreover, among the total 105,209 TOMS $O_3$ observational sites in the given domain, there are 76,118 observational sites for $S_I$ and 26,111 for $S_{II}$, which together occupy about 97.2% of the total number of observations. There are only 2980 wild points, which is only 2.8% of the total number of points. Therefore the two regime regression models not only

![Figure 5](image1.png)

**Figure 5.** Observational sites of TOMS $O_3$ for Hurricane Erin on 9 September 2001. The red dots are points in regime $S_I$, The black triangles are points in regime $S_{II}$. The green pluses are wild points (regime $S_{III}$). (a) Regression parameters are obtained with all data from 4 to 17 September, and (b) regression parameters are obtained from 4 to 8 September; that is, data up to the preceding date are used.

![Figure 6](image2.png)

**Figure 6.** Correlation between TOMS ozone and MPV and the standard error of the estimates of linear regression models with all data (corr-T and STDE-T), data in $S_I$ (corr-I and STDE-I), and data in $S_{II}$ (corr-II and STDE-II). (a) Regression parameters are obtained with all data from 4 to 17 September, and (b), except for the first day, i.e., 4 September, all data 1 day preceding that date are used. On 4 September, data from particular date are utilized.
improve the regression quality, but also make use of more TOMS $O_3$ observations compared to the whole domain regression model (1). It is expected that TOMS $O_3$ will have a larger impact on the environmental flows of tropical storms using two regime-dependent regression models for TOMS $O_3$ assimilation.

[25] Relationships between $O_3$ and MPV with and without categorizing data into regimes $S_I$ and $S_H$ for all 12 storms listed in Table 1 are shown in Figure 8. Correlations between the two variables are significantly improved when data are grouped into two different regimes for all storms (Figure 8a). There are usually more data points in regime $S_I$ than in regime $S_H$ (Figure 8b). As in the case of Hurricane Erin, only a small fraction of $O_3$ observations is removed from regression calculations for each individual storm. Figure 9 presents results of regression coefficients and the corresponding STDEs for all 12 storms. Values of both the slope and intercept of the regression models for regimes $S_I$ and $S_H$ are case-dependent. However, it is found that the intercept of the regression model in regime $S_I$ ($S_H$) is consistently larger (smaller) than that without regime separation. A similar trend is not found with the slope calculation. Compared to STDEs without regime separation, the STDEs for both regimes $S_I$ and $S_H$ are reduced by at least 50% for all storms.

4. TOMS $O_3$ Distributions Within Hurricanes

4.1. Observed Local Maxima of TOMS $O_3$ at Hurricane Eye Regions

[26] It has long been speculated that the tropopause rises gradually with the approach of the center of a hurricane [Koteswaran, 1967]. A hurricane model by Riehl [1954] also depicts the tropopause as a high dome near the 100-hPa level over the storm’s core. This model may be true for hurricanes during their initial developing stage, when the atmospheric motion is dominated by warm and moist air being lifted upward and the tropopause rises within the central region of hurricane. However, when a hurricane is well formed, a subsidence flow, evidenced by a clear hurricane eye seen on infrared satellite pictures, is often found at the center of the hurricane. Hence the claim that the tropopause over a hurricane forms a dome is therefore in question.

[27] Penn’s [1965] study was most likely the first study which indicates the increases of ozone concentration within the hurricane eye. The conceptual model proposed by Rodgers et al. [1990] also suggests that ozone-rich air
should be found in the hurricane center, though their mean Nimbus-7 TOMS $O_3$ for 53 western Atlantic tropical cyclone observations did not reveal this [see Rodgers et al., 1990, Figures 15, 20–24]. With the advancement of remote sensing techniques, observations can be obtained with higher resolutions and better quality. Compared to Nimbus-7 TOMS, the latest EP/TOMS instrument improves not only the horizontal resolution, but also the coverage of observations. The highest possible horizontal resolution of the level-2 raw non-gridded along-track TOMS total ozone data set is about 40 km, while the Nimbus-7 level 3 gridded TOMS $O_3$ data set is on a 1° latitude by 1.25° longitude resolution with some smoothing algorithm. To illustrate the difference with and without the smoothing algorithm, the total ozone distribution within the central region of Hurricane Erin on 12 September 2001 is shown at two resolutions in Figure 10. In Figure 10a, the level-2 raw non-gridded along-track total ozone data set is used, while in Figure 10b, the smoothed gridded data set obtained by Cressman analysis method with a horizontal resolution of 45 km is used. It is seen in Figure 10a that the hurricane center is generally surrounded by low values of total ozone, representing strong upward lifting of the atmosphere. At the center, there is a region of slightly larger values of total ozone. However, this local maximum of total ozone at the hurricane center is not seen in smoothed gridded total ozone data, as shown in Figure 10b. The local maximum values of total ozone at the center of Hurricane Erin indicate a
downward subsidence of the stratospheric atmosphere within the central region of the hurricane. The east-west cross section of potential vorticity across the center of Erin (see Figure 11), derived from the NCEP analysis data set, further confirms that these ozone maxima exist due to an intrusion of the ozone-rich stratospheric air into the core of the hurricane. The conceptual total ozone/tropical cyclone model of Rodgers et al. [1990] is thus substantiated by EP/TOMS level-2 non-gridded along-track $O_3$ observations.

[28] Compared with the NOAA-12 AVHRR 3 channel color composite of Erin (see Figure 12), it is found that the spiral band features can also be captured by TOMS $O_3$ observations in Figure 10. However, we should also realize the accuracy problem of TOMS $O_3$ retrieval when there is thick cloud coverage. It is known that the ozone below the

Figure 10. TOMS $O_3$ distributions within the central region of Hurricane Erin on 12 September 2001 with (a) level-2 raw data of EP/TOMS ozone and (b) gridded EP/TOMS ozone with a horizontal resolution of 45 km.

Figure 11. NCEP analysis of (a) the SLP at 1500 UTC 12 September 2001 and the east-west cross line AB and (b) the east-west cross section of PV across the center of Hurricane Erin (38.0°N, 62.1°W) along the line AB. The unit for PV is PVU. The contour interval is 0.5 PVU.
clouds is not observed, and thereby total ozone measurements must be corrected. The correction is done by adding a climatological profile of tropospheric ozone below a cloud at a given height [McPeters et al., 1998]. Although the fraction of cloud cover can be obtained from the TOMS ultraviolet reflectivity measurements, the cloud height based on climatology is questionable. When deep clouds associated with tropical cyclones are present, the underestimation of cloud height may in turn result in an underestimation in the TOMS-observed total ozone amount [Newchurch et al., 2001]. A careful examination of Figure 10 reveals that there are some small “dots” in the east side of the circular eyewall (purple color) and within the spiral bands (cyan color) characterized by relatively lower total ozone concentration (about 5–10 DU lower) than their nearby points. These relative low total ozone dots correspond well to the high reflection parts in the visible picture (Figure 12). They probably result from an underestimation of TOMS ozone due to the high reflectivity of clouds and a cloud top that was much higher than the climatological cloud pressure used in the TOMS O₃ retrieval algorithm. However, as indicated by Rodgers et al. [1991], it is the three-dimensional transport processes near the tropopause, not the tropospheric ozone, that mostly contribute to the TOMS-observed total ozone pattern. Hence we believe that EP/TOMS total ozone observations reflect the general features of tropical storms reasonably well.

4.2. Determining Upper Tropospheric Hurricane Center From TOMS O₃ Data

[29] Accurate estimates of the center of a tropical cyclone are always important in storm analysis and prediction. The
centers of a hurricane may differ between levels, owing to vertical shear and trochoidal oscillations within phases [Nolan and Montgomery, 2001]. Many methods are employed to obtain the center of the storm with various purposes. For example, ship or buoy observations provide the center of a storm at the surface, aircraft reconnaissance observations may be used to determine the center of a storm from the lower to the upper troposphere, and satellite infrared imagery provides the center of storm in the lower to middle level troposphere, while satellite visible imagery provides the center of storm in the upper troposphere. However, none of these observations are sufficient to determine hurricane centers near the tropopause, due to the inaccessibility of aircraft and a lack of water vapor and clouds in this region of the atmosphere. TOMS O$_3$ observations may be a good source of information for identifying the center of storm near the tropopause. A comparison between the TPC (Tropical Prediction Center) best track positions and the position of the local maximum of total ozone within the central region of Hurricane Erin is given in Figure 13a. It is shown that before the strong intensification of Erin, the deviation of the local maximum of TOMS O$_3$ to the center of the hurricane is relatively large. This may be caused by the fact that before the formation of Hurricane Erin, the upper atmosphere over the hurricane center is dominated by updrafts due to direct thermal convection, while a systematic subsidence of stratospheric air into the center of the hurricane is either not initiated or is not of a large enough scale to be resolved by TOMS O$_3$ observations. It is also possible that during its deepening stage, Hurricane Erin is either relatively shallow or tilted vertically. When Erin reached its mature stage, the position of the low-pressure center determined by the best track stays close to the local maximum of total ozone. The actual distance between the best track and total ozone maximum point is less than 20 km (see Figure 13b). During the decaying stage, the maximum total ozone departs from the best track again, probably for the same reasons discussed in the development stage.

[36] Figure 14 shows the daily variation of the north-south profiles of TOMS O$_3$ across the center of Hurricane Erin. The raw TOMS O$_3$ is first interpolated onto the grid points, with a spacing of 15 km to its nearest site value.
Next, a three-point smoothing is applied to obtain the profiles of TOMS $O_3$. It is shown that during the formation stage of Erin (6, 8, and 9 September), the storm center is characterized by a total ozone low. In the mature stage (from 10 to 13 September), the center correlates well with a local maximum found nearby. The hurricane center is once again characterized by a total ozone low when the hurricane starts to decay on 14 September.

Similar results regarding the relationship between TOMS $O_3$ minima and maxima and the best track are found with all the hurricanes and typhoon listed in Table 1. The averaged deviation of the local maximum of TOMS $O_3$ to the best track for mature hurricanes is about 30 km, which is well within the range of the best track error. This may also reflect the weak vertical shear in the mature stage of the hurricane. It is anticipated that the set of TOMS $O_3$ observations could be used as a valuable source of information for describing upper atmospheric flow conditions within hurricanes.

4.3. Total Ozone Variation and Hurricane Intensity Changes

The daily variation of total ozone within a hurricane is related to the strength of the subsidence of the ozone-rich stratospheric air. A decrease of total ozone amount within a hurricane, which pushes the tropopause higher, implies an intensification of deep convection. An increase of the local maximum of the total ozone amount in the core area of the hurricane indicates an enhancement of subsiding stratospheric air into the troposphere. TOMS ozone variations in both regions could be used as indices reflecting hurricane intensity changes.

Figure 15 shows a daily variation of the minimum value of TOMS $O_3$ selected from a $16^\circ \times 16^\circ$ rectangle centered at Hurricane Erin’s center based on the TPC best track estimate. Data are not plotted on 7 and 9 September due to poor viewing angles of TOMS when Erin is scanned. In general, the minimum value of total ozone decreases (increases) as Hurricane Erin intensifies (weakens). Similar results are found for the other hurricanes listed in Table 1.

In order to gain a better insight into the daily variation of TOMS $O_3$ distribution within the hurricane, the radial total ozone profiles are calculated based on the gridded TOMS $O_3$ data (Figure 16). On 6 September, when Erin was weakened by vertical wind shear, the radial profile of TOMS $O_3$ is rather flat. With the intensification of Erin, the radial gradient near the hurricane center becomes larger. The radial profile of TOMS $O_3$ becomes sharpest at 1500 UTC 9 September, right before Erin reached its maximum intensity.

4.4. Correlations Between TOMS $O_3$ and Geopotential Height at 340 K Isentropic Surface Within a Hurricane

In the prediction of a hurricane, the fine structure of the hurricane, together with the correct large-scale environmental field, and the initial structure of the hurricane itself, is vital. However, owing to sparse observations over the open sea and coarse resolutions of large-scale analysis fields, it is often difficult to discern these fine structures of the storm and its intensity. The analyzed hurricane could also be misplaced. These aspects are especially true before a hurricane reaches a certain intensity. A useful procedure for initializing a hurricane prediction model is to plant a synthetic vortex into the large-scale field. Zou and Xiao [2000] developed a 4D-Var bogus data assimilation (BDA) scheme, which places a bogus SLP field into the model, while other fields are generated under the constraint of the model dynamics and physics. The bogus SLP that is assimilated into a hurricane prediction model is obtained by the Fujita’s formula, with required parameters derived from the TPC best track analysis. In this section, ways of deriving hurricane bogus fields from TOMS $O_3$ data are explored.

To establish a basis for deriving the small-scale structures of a hurricane from TOMS $O_3$ observations, the meteorological quantities that are well correlated with TOMS $O_3$ within a hurricane need to be known. It is found that among other quantities, $\Phi_{340K}$ is well correlated with TOMS $O_3$.
Figure 17. (a) Daily evolution of the correlation between TOMS $O_3$ and $\Phi_{340K}$ within a 500 km radius of the center of Hurricane Erin. (b) Scatter diagram of the correlation between TOMS $O_3$ and $\Phi_{340K}$ with respect to latitudes of hurricane centers for the selected storms with good viewing angles.

$O_3$. Figure 17a shows a daily variation of the correlation between TOMS $O_3$ and $\Phi_{340K}$ within a radius of 500 km. The correlation remains as high as 0.8. The strong correlation between TOMS $O_3$ and $\Phi_{340K}$ is found to be evident for almost all the storms listed in Table 1 (Figure 17b). The two storms for which the correlation between $O_3$ and $\Phi_{340K}$ is lower than 0.7 are found to be caused by the lack of a well-defined low center in the NCEP analysis of $\Phi_{340K}$.

In order to compare structural differences between $O_3$ and $\Phi_{340K}$, we show in Figure 18 horizontal distributions of SLP and $\Phi_{340K}$ from NCEP analyses as well as TOMS $O_3$ on 6, 8, and 10 September 2001, respectively. The NCEP analysis shows a southward misplaced SLP low at 1500 UTC 6 September (Figure 18a) and a very weak low center of the geopotential height in the upper troposphere (Figure 18b). However, a well-defined low total ozone pattern is seen southeast of the total $O_3$ trough in TOMS $O_3$ (Figure 18c). This corresponds to a tropical cyclone located to the southeast of an upper-tropospheric trough, which is expected to favor for the intensification of Erin [Rodgers et al., 1990]. At 1500 UTC 8 September (right before Erin became a hurricane), the surface low described by the NCEP analysis data set is about 13 hPa weaker than the observed low (Figure 18d). It is difficult to associate it with a storm which would soon evolve into a hurricane 9 hours later. The $\Phi_{340K}$ shows a similar weak geopotential height low near the tropical storm center (Figure 18e). However, a total ozone low near the center of the storm is very well defined (Figure 18f). Moreover, both the total ozone low center and the downstream total ozone trough become deeper than those on 6 September, clearly indicating an intensification of the storm. At 1500 UTC 10 September, although the analysis SLP is still too weak (Figure 18g), the upper atmospheric flow pattern is captured by both $\Phi_{340K}$ and TOMS $O_3$ (Figures 18h and 18i). Moreover, TOMS $O_3$ exhibits some fine structures, especially the southeastward tilt due to the intensification of outflow jet (Figure 18i).

5. Summary and Conclusions

The EP/TOMS total ozone and NCEP analysis data are employed in the investigation of the relationship between TOMS $O_3$ and various meteorological quantities within and around a hurricane. It is found that the correlation between TOMS $O_3$ and MPV derived from NCEP analysis data decreases greatly when an intensifying hurricane is present in the given domain. A new algorithm is developed to improve the correlation between the two quantities. This algorithm separates TOMS $O_3$ data into two regimes and develops a linear regression model for each regime. Both the correlation between the TOMS $O_3$ and MPV and the standard error of the simulated $O_3$ from MPV are greatly improved in two regimes, which together contain more than 97% of the total ozone observations in the domain. A small portion of TOMS $O_3$ observations (<3%) is identified as outliers and is eliminated from the calculations.

Over a few hundred kilometers, the area of the hurricane is characterized by a low column ozone content. An increase in hurricane intensity corresponds to a decrease of TOMS $O_3$ content within the storm. Within this low-ozone area, a hurricane eye can be clearly seen in TOMS $O_3$ data, corresponding to a local maximum of TOMS $O_3$ embedded in a larger region of low ozone content. For the 12 chosen storms, the mean distance between the local maximum of TOMS $O_3$ and the TPC reported hurricane center is less than 30 km during their mature stages.

Within a hurricane, TOMS $O_3$ is found to be highly correlated with the geopotential height on the 340 K...
isentropic surface in the upper troposphere. This finding provides a possibility for constructing spatial distributions of $\Phi_{340K}$ from TOMS $O_3$ data and using them for hurricane initialization. The constructed $\Phi_{340K}$ fields contain valuable structural information of a hurricane that the NCEP reanalysis data set often lacks due to its coarse resolution, especially during the developing stage of a storm.

The strong correlations between TOMS $O_3$ and $\Phi_{340K}$ within a hurricane, and those between TOMS $O_3$ and regime-dependent MPV, provide a way of making use of TOMS $O_3$ observations for hurricane prediction. Within a hurricane, TOMS $O_3$ can be used to formulate bogus $\Phi_{340K}$. It is anticipated that a hurricane initialization procedure which adds a bogus $\Phi_{340K}$ will be more effective than the 4D-Var BDA scheme used by Zou and Xiao [2000], owing to the additional information on the upper level atmospheric motion available from TOMS $O_3$ observations. A well-defined horizontal distribution of TOMS $O_3$ for developing storms allows for a TOMS $O_3$ hurricane initialization procedure to improve the prediction of developing hurricanes. On the large scale, the strong correlation of TOMS $O_3$ to MPV in two separate data regimes described in

Figure 18. Distributions of (left column) SLP, (middle column) $\Phi_{340K}$, and (right column) TOMS $O_3$ for Hurricane Erin at 15 UTC on (top row) 6 September, (middle row) 8 September, and (bottom row) 10 September.
section 3.2 can be used to better define the hurricane environmental flow features. The proposed strategy of improving both the initial structure of a tropical cyclone and its environmental flow by TOMS O$_3$ data is being tested, and results will be presented in a future paper.

[42] Acknowledgment. This research is sponsored by National Aeronautics Space Administration (NASA) under the research project grant NAG5-11067.

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