Episodic Total Ozone Minima and Associated Effects on Heterogeneous Chemistry and Lower Stratospheric Transport

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A description of the January 31, 1989, ozone minhole over Stavanger, Norway, is given on the basis of three-dimensional model simulations. This minihole is typical (though of large magnitude) of many transient events in the lower stratosphere that arise because of cyclonic-scale disturbances in the troposphere. The ozone reduction is a short-lived reversible dynamical event. However, through heterogeneous chemical processes there can be a significant transfer of chlorine from reservoir molecules to active radicals. This chemically perturbed air is defined as processed air, and it is found that a single event can produce enough processed air to reduce the HCl in the entire polar vortex. Chemical processing on clouds associated with transient events is shown to be a major source of processed air in the polar vortex in December before background temperatures are cold enough for more uniform heterogeneous conversion. In the model, intense cyclonic scales propagating close to the vortex edge and large planetary wave events (especially stratospheric warmings) are the major mechanisms of extra-vortex transport. Only a small amount of processed air is found outside of the polar vortex. The processed air is a strong function of longitude, and it is virtually excluded from the Pacific Basin.

INTRODUCTION

Transient depressions of total ozone were first described as miniholes in the southern hemisphere Total Ozone Mapping Spectrometer (TOMS) data [Newman et al., 1988]. These disturbances of several tens of DU's (Dobson units = \(2.67 \times 10^{16}\) molecules cm\(^{-2}\)) were found to be associated with tropospheric anticyclones and had time scales of a few days. On January 31 and February 1, 1989, a minihole formed over Scandinavia. This minihole received some notoriety because it occurred during the Airborne Arctic Stratosphere Expedition (AASE). During this minihole event, total ozone amounts as low as 174 DU were observed by TOMS. (Previously, a value of 146 was reported with version 5 TOMS data. This paper uses the internally calibrated version 6 TOMS data [see Herman et al., 1991]. This was the lowest value observed during AASE.)

Other northern hemisphere miniholes that have received attention include the January 24, 1989, event [e.g., Poole et al., 1990; Jones et al., 1990] and the February 6, 1990, event [e.g., Hofmann and Deshler, 1990]. These events are all associated with meteorological disturbances called anticyclones, primarily of tropospheric origin. Anticyclones are high-pressure systems. During the passage of an anticyclone there will be both horizontal and vertical movement of ozone. While both the horizontal and vertical components are important [e.g., McKenna et al., 1989], conceptually the minihole can be imagined as the lifting of ozone-poor tropospheric air upward as the anticyclone passes. By continuity, there will be divergence of ozone-rich air out of the column, and there will be a reduction of the ozone column. This uplifting also produces lower temperatures and can lead to cloud formation. These clouds provide surfaces for heterogeneous processes in the lower stratosphere.

Because of the presence of high clouds, questions have risen as to the accuracy, or even the reality, of miniholes in the TOMS data. The TOMS inversion algorithm makes a climatological assumption about clouds and cloud heights. The algorithm is known to be deficient in the presence of high clouds, especially at high solar zenith angles [Klenk et al., 1982]. The Ozone Processing Team is actively investigating the accuracy of the TOMS algorithm when clouds are present. (The Ozone Processing Team is responsible for processing and reprocessing and quality control of TOMS and Solar Backscattered Ultraviolet (SBUV) ozone data. It is currently headed by Richard McPeters. They have recently produced the version 6 TOMS data which are internally consistent [see Herman et al., 1991]. One of us (R.S.S.) is on this team.) They find that the errors can be tens of DU's when the optical thickness of the clouds is large and much smaller at smaller optical depths [Torres et al., 1991]. Hofmann and Deshler [1990] have presented sondes that suggest large errors in the TOMS observations during miniholes.

Our research group has undertaken the task of producing realistic three-dimensional (3D) simulations of constituent variability during AASE. The simulations are global, and it is a goal of the effort to place the localized measurements taken during AASE on a global perspective. The model has proven to simulate miniholes with characteristics similar to those observed in TOMS data. This suggests that the miniholes are a real feature in the ozone field and not entirely an artifact of the inversion algorithm.

McKenna et al. [1989] presented diagnostic analyses of southern hemisphere miniholes, associated cloud formation, and exchange of vortex air with extra-vortex air. They confirmed that the miniholes were dynamically forced by tropospheric anticyclones and that there was only little exchange with air from outside the vortex. The satellite aerosol data showed the formation of extensive layers of polar stratospheric clouds as the anticyclone passed. With the aid of trajectory analyses, it was determined that a large amount of the air in the vortex could pass through these clouds and possibly experience heterogeneous chemistry.
McKenna et al. concluded that mass exchange between air in the vortex and out of the vortex over the course of the spring "would be 3–5% of the mass of the depleted region." They emphasized that their calculated transport was probably a lower limit.

Our study investigates many of the same issues as McKenna et al. [1989] except for the northern hemisphere. It builds on their results using the 3D model as a tool. The 3D model allows for clear exposition of the dynamics that produce the minihole, including the vertical velocity field. By the design of special experiments, it is possible to reveal when and where processed air is formed and how the air is then distributed. The simulations are seasonal in length and have been performed for both 1979 and 1989 winters.

Following a brief discussion of the model and recent alterations to its transport algorithms, the structure and dynamics of the late January 1989 event are discussed. The model simulation is compared to TOMS data and AASE data. Based on the success of this simulation and on the success of our chlorine simulations [Douglass et al., 1991; Kaye et al., 1991], the model is then used to determine the effects of anticyclonic events of tropospheric origin on the ozone and chlorine budget. The chlorine study is centered on the production of processed air, which is defined as air that has had HCl reduced by heterogeneous chemistry. Finally, the production and transport of processed air to latitudes outside of the polar vortex are examined.

**The Model**

The modeling technique and earlier results from the AASE simulations have been described by Rood et al. [1989], Kaye et al. [1990, 1991], and Douglass et al. [1991]. The most extensive report, Rood et al. [1991], demonstrates by comparison with satellite and ground-based data that realistic simulations for the entire winter are realized. Basically, in this modeling approach an offline chemistry and transport model (CTM) is driven by winds from the forecast stratospheric assimilation system STRATAN [Rood et al., 1990a; Steenrod et al., 1992]. The CTM was initialized on December 28, 1988, and December 1, 1978, using the technique of Douglass et al. [1990].

It is emphasized here that the dynamics of wind and temperature are from the STRATAN system. In data assimilation a dynamical general circulation model is used as an analysis tool to process conventional and satellite data. Two periods have been analyzed: December 28, 1988, through March 31, 1989, and December 1, 1978, through May 31, 1979. Because STRATAN winds and temperature are used, this is an attempt to model constituent transport and chemistry for specific time periods. Also because STRATAN data are used, the geographical location of temperature structures should be accurately represented. Similarly, the magnitude and time fluctuation of the dynamic variability are realistically represented. A comparison of STRATAN temperatures to radiosondes is given by Rood et al. [1990a].

There have been two major changes to the CTM since the earlier work. First, the transport algorithm in the horizontal directions has been changed to that of van Leer [1974]. This grid point scheme requires no filling but is diffusive in the sense of shape-preferential schemes [Rood, 1987; Allen et al., 1991]. In order to reduce the impact of this self-limiting diffusion, the CTM is run at higher resolution than previously (2.5° longitude, 2° latitude).

Furthermore, because of the vigorous cascade of constituent variability to high wave numbers by differential advection, it is justified to use a higher resolution CTM than dynamics model. An essential ingredient of this modeling approach is to use the relatively high-resolution CTM to provide a mechanism of advective cascade and mixing. The monotonicity algorithm assures that the mixing takes place on only the smallest resolvable scales. The success of these simulations in representing large-scale structures implies that the details of the small-scale structure are not a crucial part of the transport process. This suggests that once the constituents are spread to a certain scale, mixing is rapid and local. It must be emphasized that these results do not say that small-scale structure is unimportant, only that a physically meaningful representation of this structure is necessary. This has been discussed more fully by Rood et al. [1991] and Rood [1991].

The second major change involves the vertical formulation of the model. The model extends from the ground to 0.4 hPa. In the stratosphere the resolution is close to 3.5 km, and in the troposphere the resolution is of the order of 2 km. This resolution is coarse and, without careful attention to the numerics, very profoundly affects the calculations.

Therefore, Prather's [1986] advection scheme has been incorporated for the vertical transport. Because this scheme can resolve an order of magnitude across one grid box, this highly accurate scheme reduces the impact of the low vertical resolution. Prather's scheme requires too much storage to run routinely in three dimensions. Along with these transport algorithm changes, the method used to calculate the vertical velocity has been altered to force continuity with the transport algorithm numerics. This, or some similar constraint, is required of all constituent advection schemes in order for them to hold together numerically [see Allen et al., 1991]. Since vertical velocity is in general a diagnostic in general circulation models, this numerical consistency requirement has little impact upon the interpretation of the results. The vertical velocity is not dependent on the distribution of any particular constituent. Despite the use of Prather's scheme, the coarse vertical resolution remains a problem, and improved vertical resolution (1 km) is a major priority.

**The January 31, 1989, Minihole**

**Ozone Behavior**

Figure 1 shows longitude-latitude maps of TOMS total ozone and model total ozone (Mout is model output) from January 30 through February 2, 1989. The areas void of contours in the TOMS plots are due to polar night or missing data. The evolution of the total ozone in the model shows many similarities to TOMS. On January 30 a weak center of low total O$_3$ has formed north of 60° just west of Greenwich (0°E). On January 31 there has been an intensification of the low total O$_3$ and the formation of the minihole centered 10°-20° east of Greenwich. The TOMS minihole appears slightly deeper and more confined. On February 1 the model minihole has partially filled in, and the TOMS minihole has deepened. On February 2 the minihole has decayed, and high total ozone is present in the west. The magnitude and spatial structure of the TOMS data and Mout on January 30 and February 2, before and after the event, are significant.
This suggests that the model representation of the event on January 31 and February 1 might quantify some real differences between the measured ozone and actuality, particularly on February 1.

Figure 2 shows vertical profiles of model ozone and temperature at the point nearest the ozone minimum on January 30 and 31 (lowest minimum) and February 1. Therefore these profiles are taken following the propagation of the minihole. The profile on January 31 shows that ozone has been removed from all altitudes below 25 km and that by February 1 there has been significant restoration of the O₃ profile.

The temperature profiles at the center of the minihole show a greater than 5 K drop in temperature between January 30 and 31 in the lower stratosphere. There has been some recovery by the February 1. Both the O₃ and temperature behavior are consistent with the uplifting caused by a passing anticyclone. The temperatures become cold enough that extensive cloud formation is possible, and clouds were observed during AASE [Gandrud et al., 1990; Browell et al., 1990b; Pitts et al., 1990].

During AASE, ozonesondes were launched frequently from Lerwick, Scotland (60°N, 1°W) [Torres and Jorgensen, 1989]. It is interesting to consider the temperature data from these sondes as contrasted to the operational temperature data. Between January 30 and 31, the operational sonde data show a drop in temperature of the order of 4 K, consistent with the temperature drop in STRATAN. The temperatures that were measured with ozonesondes show a much larger temperature drop of the order of 10 K. These ozonesonde temperatures are not part of the operational data base and therefore are not incorporated into STRATAN. These colder temperatures could be the signal of a disturbance more intense than that measured by the operational data and hence as simulated by STRATAN. On the other hand, the cold temperatures could simply represent a localized event of little meteorological consequence. If they did, in fact, represent an organized circulation that STRATAN missed, then perhaps the Mout on February 1 would have been lower and closer to the TOMS observations (see Figure 1).

On January 30 and 31 the minihole propagated over Lerwick. The Lerwick ozone data offer not only a way to
check the model performance, but also offer a check on the TOMS data during the development of the minihole. Figure 3 shows the Lerwick total ozone data from sondes and the TOMS data from the point closest to Lerwick in the gridded data (60°N, 2.5°W). Between January 26 and 30 the differences are never more than 4 DU. After February 2 the agreement between TOMS and Mout is more erratic. From January 31 through February 2, TOMS is deficient by 18, 17, and 12 DU. Even though the Lerwick data and the TOMS data might be biased during this period, the Lerwick data do confirm the formation of a total ozone minimum. Unfortunately, at the time the minihole is most intense, it has moved east of Lerwick.

Figure 4a shows a time series of O₃ partial pressure over Lerwick for most of the AASE period. It is constructed from the data returned from 28 ozonesondes launched between January 10 and February 13, 1989. The vertical extent of the minihole is evident on January 31 and February 1 below 50 hPa. The transience of the event is indicated by the rapid recovery of the ozone partial pressure in 4 days. Figure 4b is
a time series from the same period for the model. Mout was taken on only the same days that sondes data were available. With its relatively poor vertical resolution, the model cannot imitate the small structure in the sondes data, but the ozone in the model is seriously depleted below 60 hPa on January 31. There is also an indication of the earlier event on January 24 in both the data and the Mout.

More detailed representation of the model performance compared with the sondes data is given in Figure 4c, which shows the individual sondes for January 11–13. As expected, the model cannot represent the small-scale structure explicitly. However, both the Mout and the observations show a bending of the ozone profile between 200 and 400 hPa, so that much more ozone is present at lower altitudes on January 12 than either January 11 or 13. Even though the model captures many of the features of the sondes data in Figure 4, obvious inadequacies remain. Two important ones are the model’s inability to represent the confused structure that is often present between the 75- and 100-nbar contours, and the extent to which tropospheric disturbances penetrate the stratosphere. The impact of these two inadequacies is important for many applications but is not believed to be crucial for the current study.

There is also vertical profile information available from flights that the DC-8 flew out of Stavanger, Norway (59°N, 5.5°E), on January 31 and February 2. The DC-8 flew directly under the minihole on January 31. Figure 5 shows Mout and differential absorption lidar (DIAL) O₃ data [Browell et al., 1990a] from these flights. The DIAL data have much more structure than is possible for the model to represent. However, there is a basic feature present in both the Mout and the observations. This feature is most easily seen by transposing the 2-ppm contour from February 2 to the January 31 plot. In both the data and the Mout the 2-ppm contour has been displaced downward on February 2. The displacement is about the same in the atmosphere and the model and corresponds to about 1 contour interval, 0.5 ppm.

The behavior of the model and data confirms the reality of the minihole. Considering the budget in a column centered above the ozone minimum, the biggest changes in the
column occur between 1200 UT on January 30 and 1200 UT on January 31. The largest changes are in the upper troposphere and lower stratosphere, where more than 80% of the total ozone decrease occurs in the layers between 200 and 30 hPa. However, there are decreases in the column O₃ thickness to altitudes greater than 10 hPa (~32 km).

**Dynamics of the Minihole**

Figure 6 shows the geopotential height deviations from the zonal mean on January 31. Both latitude- and longitude-height sections are shown. From the ground to the lower stratosphere there is little longitudinal tilt, but there is a distinct tilt to the north with increasing latitude. This anticyclonic disturbance is consistent with the description of southern hemisphere miniholes [Newman et al., 1988; McKenna et al., 1989]. The height maximum is somewhat to the south and west of the center of the total ozone minimum. In the middle and upper stratosphere, there is a tremendous geopotential low associated with the end of a wave 1 warming [Steenrod et al., 1992].

The wind fields responsible for the minihole are shown in Figure 7 on the 150-hPa surface. The panels show the zonal velocity (u), both with and without the zonal mean removed, the meridional velocity (v), the vertical velocity (w = d [-H log (p/p₀/dt)], and the model column ozone. The total u field shows winds of the order of 60 m s⁻¹, consistent with the strong winds measured by the radiosondes. The anticyclonic circulation is clearly visible. Furthermore, there is vigorous upward motion to the north and the west of the center of the circulation. There is downward motion to the south and east. The maximum magnitude of the vertical velocity is 11 cm s⁻¹, and there are large areas where the vertical velocity is greater than 2 cm s⁻¹. The anticyclone contains a fully 3D, internally confined circulation.

HETEROGENEOUS PROCESSING

**Formation of Processed Air**

Figure 1 shows that on January 30 and February 2 the model has rendered a reasonable representation of the ozone field. At the altitudes of the total ozone disturbance, the model ozone chemistry is very slow compared to this 4-day span. Therefore it is safe to conclude that to first order the minihole is primarily a reversible dynamical event. The presence of clouds, however, might enhance processing of chlorine reservoir species to reactive species. Furthermore, the transient colder temperatures could cause the formation of water particles large enough to fall from the stratosphere, resulting in denitrification through the scavenging of nitrogen-containing compounds. Gandrud et al. [1990] discuss dehydration during the event. This section will address the formation of heterogeneously processed air.
A simple representation of heterogeneous chemistry has been incorporated into the 3D model to evaluate the conversion of HCl to reactive chlorine. Heterogeneous processing is implemented by an increase in the HCl loss to a 3-day time constant at or below a prescribed temperature that is a function of pressure. The threshold temperatures on pressure surfaces are 199 K, 175 hPa; 197 K, 91 hPa; 195 K, 53 hPa; and 192 K, 31 hPa. These criteria are based on Hansen and Mauersburger [1988]. There is no consideration of chemical processes occurring on background sulfuric acid aerosols.

The behavior of HCl with heterogeneous chemistry in the 3D model has been reported by Kaye et al. [1990] and more recently with the new transport scheme in Douglass et al. [1991] and Kaye et al. [1991]. Douglass et al. [1991] show that the geographical distribution of the HCl destruction is similar to the ClO measurements during the AASE ferry flights. Therefore, it is concluded that the model provides a realistic simulation of the location of air that has had reactive chlorine enhanced through heterogeneous processing.

Figure 9 shows differences of the profiles of both HCl (gas phase chemistry only) and DHC1 (heterogeneous chemistry) between January 30 and February 1 following the center of the ozone minihole (same location as Figure 2). By February 1 the HCl profiles have largely recovered to values seen prior to the minihole event. The DHC1 profile shows profound reduction of up to 60% in the 20- to 25-km layer. Significant local conversion by heterogeneous processes of HCl to potentially reactive Cl has occurred in the minihole.

The amount of air processed in these events can contribute substantially to the processed air in the polar vortex. Figure 10 illustrates this point. This figure is for an experiment run with winds for December 1978 to March 1979, and represents the first major processing event of the winter at 53°S.
hPa. It is coincident with a passing anticyclone and the reduction of temperatures below the threshold values necessary for processing. Processed air is defined as the ratio \( \text{DHCI/HCi} < 1 \). Prior to December 25, 1978, there is little evidence of processed air in the model. Then on December 25 an event begins, and \( \text{DHCI/HCi} \) dramatically dips below 1. Over the next 5–7 days, air is processed over the North Atlantic, travels eastward, and ultimately encircles the pole. At 30 hPa, processing does occur earlier, but it does not propagate to the lower altitudes. This paper will focus on the 53 hPa results, which are closer to the ER-2 flight levels. The 30 hPa processing will be discussed later.

Figure 11 shows that the vortex is largely filled with air that has seen some level of processing. The entire area with potential vorticity values \( >2.8 \times 10^{-5} \text{ K m}^2\text{ kg}^{-1}\text{ s}^{-1} \) contains some processed air. The vortex is not homogeneously mixed, and a definitive track of more highly processed air is seen moving downstream from the North Atlantic/Greenland/Scandinavian areas. As time proceeds, the processed air remains confined to the polar vortex, and ultimately the area with vorticity values \( >2.0 \times 10^{-5} \text{ K m}^2\text{ kg}^{-1}\text{ s}^{-1} \) contains highly processed air. There is little obvious spread outside the vortex.

In the minihole event of January 31, 1989, the signal of processing and the distribution of the processed air are not as clear as in Figure 10. The major reason is that the minihole processing occurs on a background of highly processed air that has formed during the cold January temperatures. Movies of the model output suggest, however, that the minihole processes a region of air that was largely unprocessed prior to January 31. Furthermore, the movies suggest that the processed air is ultimately confined to the polar vortex. Pitts et al. [1990] show that clouds were observed as far south as 50°N during this event. Therefore it is perhaps surprising that the newly processed air is confined to the polar vortex. This will be examined more quantitatively in the next section.

In order to examine the effect of the minihole more carefully, a special experiment was performed. Experiments and other special definitions are summarized in Table 1. In this experiment the model was initialized with gas phase HCl on January 27, and the heterogeneous chemistry was turned on. Therefore this is an attempt to reproduce the conditions of Figure 10—an episodic event occurring on a background of unperturbed air.

Figure 12 shows potential vorticity on the 450 K surface and a map of \( \text{DHCI/HCi} \) from this special experiment. Once again, most of processed air is confined to the vortex. However, the ambient temperature in the vortex is very low, and there is generalized processing. Therefore, this experiment is not as clean an event as that discussed in Figure 10.

**Fig. 8.** (a) Geopotential height (m) on the 450 K theta (potential temperature) surface. (b) The vertical velocity (cm s\(^{-1}\)) at 91 hPa. All polar projections are orthographic with latitudes drawn at 0°, 30°N, and 60°N.
Compared to Figure 11, the vortex is clearly filled to the $2.0 \times 10^{-3} \text{ K m}^2 \text{ kg}^{-1} \text{ s}^{-1}$ contour instead of just the $2.8 \times 10^{-3} \text{ K m}^2 \text{ kg}^{-1} \text{ s}^{-1}$ contour. This is indicative of the processing event occurring at lower values of potential vorticity on the edge of the polar vortex.

**Horizontal Distribution**

The exact amount of isolation from the rest of the hemisphere of the polar vortex during winter is an important problem. Either by direct transport of ozone-depleted air or by transport of heterogeneously perturbed air, conditions in the polar vortex can have an influence on middle latitude and subtropical air outside the vortex. The picture that the simple model of Juckes and McIntyre [1987] provides is a vortex of nearly complete isolation during winter.

There is little doubt that in the transition from winter to spring there is wholesale mixing of polar air with the rest of the hemisphere. Prather et al. [1990] and Grose et al. [1990] have studied the effect of dilution of the Antarctic ozone hole in this seasonal transition. The midwinter mixing with middle latitudes is much more subtle. Schoeberl et al. [1990], among others, conclude that the Arctic vortex is highly isolated. Proffitt et al. [1990] describe the Arctic vortex as a "flowing processor" that is always being replenished with ozone. The quantification of vortex/middle latitude interaction, vortex leakiness, is a problem that pushes the data and models to the limit of reliability. The degree of isolation, and its importance, is frequently a subjective measure.

Cariolle et al. [1990], using a numerical model, conclude that the Antarctic vortex is leaky. Rood et al. [1990b] conclude that, within the constraints of the Limb Infrared Monitor of the Stratosphere (LIMS) HNO$_3$ data, the Arctic vortex is basically isolated. Our experience using both spectral general circulation models and winds from the data assimilation is that there is significantly more "numerical transport" in the spectral general circulation model than in the assimilation approach. Given that the assimilation approach has had notable success in comparisons with data, an
attempt will be made to evaluate how much processed air might escape the vortex during winter.

It is difficult to define a quantitative measure to determine what is in and what is out of the vortex, partly due to the arbitrary nature of the definition of the edge of the vortex. As mentioned earlier, visual examination of the maps of processed air and potential vorticity on the 450 K surface suggests that the $2.0 \times 10^{-5}$ K m$^2$ kg$^{-1}$ s$^{-1}$ contour is a boundary, and this will be used here. Schoeberl et al. [1990] use the $2.6 \times 10^{-5}$ K m$^2$ kg$^{-1}$ s$^{-1}$ contour as the vortex boundary on the 440 K surface. The AASE data suggest that $2.8 \times 10^{-5}$ K m$^2$ kg$^{-1}$ s$^{-1}$ is a very tight definition of the vortex edge, and $2.0 \times 10^{-5}$ K m$^2$ kg$^{-1}$ s$^{-1}$ is a much weaker definition.

There is air outside the $2.0 \times 10^{-5}$ K m$^2$ kg$^{-1}$ s$^{-1}$ boundary with $\text{DHCI/HCl} < 1$, possibly caused by real transport processes, processing occurring outside the vortex, or numerical inaccuracies. There are times when the processed air in the vortex appears to simply oscillate about this boundary without definitive collocation of the vorticity and constituent boundaries. Even in this situation, however, clearly visible boundaries exist between the large regions of processed and unprocessed air. Part of this phenomenon could arise from interpolation to the 450 K surface.

In an attempt to address the question of processed air outside of the vortex, and whether or not the January 31 event resulted in processed air outside of the vortex, the following analysis has been performed. First, the 450 K surface has been restricted to latitudes north of 20øN. Then only the air with potential vorticity values $<2.0 \times 10^{-5}$ K m$^2$ kg$^{-1}$ s$^{-1}$ is considered. These restrictions generally define a rim or halo around the vortex. Within this region the demographics of the grid points are considered.

Populations are considered in three groups. These are "highly" processed air, where $\text{DHCI/HCl} \leq 0.90$, "slightly" processed air, where $\text{DHCI/HCl} \geq 0.97$, and the remaining group in between, the "moderately" processed air. These definitions are summarized in Table 1. Given all of the inaccuracies of the model, it is the purpose of the highly processed air to represent air that with some confidence has seen physically or chemically significant amounts of processing. While it is not the purpose of the slightly processed air to represent unprocessed air, any conclusions about reactive chlorine leaking at this level are completely suspect. The moderately processed air can be effectively used to prove whatever point one's preconceptions demand.

A second special experiment has been performed to study horizontal mixing. For this experiment, refer back to Figures 10 and 11 and the isolated processing event that occurred in late December 1979. Figure 11 shows the vortex containing processed air only to the $2.8 \times 10^{-5}$ K m$^2$ kg$^{-1}$ s$^{-1}$ contour.

\begin{table}[h]
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\caption{Definitions Used In Text}
\begin{tabular}{|l|l|}
\hline
\textbf{Term} & \textbf{Definition} \\
\hline
\text{DHCl} & HCl that has heterogeneous chemistry parameterization \\
\text{Vortex "halo" or "rim"} & Area on the 450 K surface north of 20øN and south of the potential vorticity contour $2.0 \times 10^{-5}$ K m$^2$ kg$^{-1}$ s$^{-1}$ \\
Slightly processed & $0.97 < \text{DHCI/HCl} < 1.0$ \\
Moderately processed & $0.90 < \text{DHCI/HCl} \leq 0.97$ \\
Highly processed & $\text{DHCI/HCl} \leq 0.90$ \\
\text{Experiment} & \\
\text{Normal 1989 run} & From Dec. 28, 1988, through March 31, 1989 (Exp 357 and Exp 367) \\
\text{Normal 1979 run} & From Dec. 1, 1978; through March 31, 1979 (Exp 356) \\
\text{Special experiment 1} & From Dec. 27, 1989 through Feb. 10, 1989, initialized with gas phase HCl, then heterogeneous chemistry is turned on; designed to test processing of 1989 minihole event as well as to help isolate transport associated with the minihole (Exp 358) \\
\text{Special experiment 2} & From Jan. 5, 1979, through Feb. 10, 1976, conservative experiment to test vortex leakiness and possible numerical effects (Exp 359) \\
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\end{tabular}
\end{table}
In this special experiment, all chemistry was turned off and the DHCl and HCl evolved conservatively after January 5, 1979. Since the processed air was initially clearly confined to the vortex, this experiment provides information on leakiness by numerical and physical transport. Under the a priori assumption that nothing should leak from the vortex physically, this test would address the numerical leakiness.

Table 2 presents the number of points outside of the vortex that are only highly processed or either moderately or highly processed as a function of vortex boundary. These values of potential vorticity traverse the edge of the vortex. Mout is chosen for two days: January 6, 1979, immediately after initialization, and January 19, 1979, just prior to the wave 1 minor warming. It will be shown below that the warming is associated with the transport of processed air to outside the polar vortex. There are normally 600–700 points outside the vortex, north of 20°N (for analysis purposes, data are stored on a 4° latitude by 5° longitude grid).

From this table there is little evidence of an increase of highly processed air outside of the vortex at any of the chosen vortex boundaries. The number of points that contain moderately processed air increases for all definitions of the vortex boundary. Under the assumption that all of the drift out of the vortex is numerical, it can be concluded that the numerical processes do not move air all the way from the interior of the vortex to the exterior. The moderately processed air indicates, however, there is some drift across the edge. For this experiment the amount of highly processed air outside the vortex is not affected by the model numerics.

In Figure 11 the processed air filled the vortex only to the 2.8 × 10⁻⁵ km² kg⁻¹ s⁻¹ contour. The processing occurred deep in the vortex, and this special experiment suggests that it remains largely confined to the vortex. More generally, however, there will be processing of air where the potential vorticity is closer to 2.0 × 10⁻⁵ km² kg⁻¹ s⁻¹. This processing occurs at the edge of the vortex, and the minihole in late January has significant amounts of associated edge processing. The results in Table 2 show that some of this highly processed edge air could indeed be transported outside the vortex by what might simply be numerical errors. However, all numerical experiments suggest that the numerical impact on the highly processed air is small.

With these numerical considerations in mind, transport of physically and chemically meaningful amounts of processed air will be studied. Five days are considered: January 3 and February 5, 1979, January 27 and February 5, 1989, from the standard 1989 experiment, and February 5, 1989, from the first special experiment to study the minihole (see Figure 12 and discussion). January 27 is the date of the beginning of the special experiment, and January 3 is 9 days after the beginning of the 1979 event discussed in Figure 10.

Figures 13a–13e show histograms of the population of the points in the halo region. The value at 93 in Figure 13, for instance, represents the number of points where DHCl/HCl is between 0.93 and 0.94. In all figures the bulk of the air is either unprocessed or slightly processed. On all days, with the exception of January 3, 1979, there is some highly processed air with values <0.90. On January 3, 1979 (Figure 13a), there is no air present with values <0.97, and essentially no processed air has escaped the vortex.

The January 27, 1989, distribution (Figure 13b) serves as a baseline prior to the minihole. Clearly, the bulk of the air has values greater than 0.98, and there is very little processed outside of the vortex. The February 5 output from the standard experiment (Exp 337, Figure 13c) shows a significantly higher percentage of the population with values outside the 0.98 range. The vast majority of the points have values >0.95. Most of the air remains in the slightly pro-

**TABLE 2. Populations of Processed Air**

<table>
<thead>
<tr>
<th>Vortex Boundary</th>
<th>January 6</th>
<th>January 19</th>
</tr>
</thead>
<tbody>
<tr>
<td>Highly Processed</td>
<td>Moderately +</td>
<td>Highly Processed</td>
</tr>
<tr>
<td>2.0 × 10⁻⁵</td>
<td>6</td>
<td>26</td>
</tr>
<tr>
<td>2.2 × 10⁻⁵</td>
<td>14</td>
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</tr>
<tr>
<td>2.4 × 10⁻⁵</td>
<td>21</td>
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</tr>
<tr>
<td>2.6 × 10⁻⁵</td>
<td>27</td>
<td>83</td>
</tr>
<tr>
<td>2.8 × 10⁻⁵</td>
<td>40</td>
<td>105</td>
</tr>
</tbody>
</table>

Fig. 12a. Same as Figure 11a for February 5, 1989, in the special experiment when no processing is allowed before January 27, 1989.

Fig. 12b. Same as Figure 11b for February 5, 1989.
Fig. 13. Histograms of the points in the halo region (points on the 450 K surface north of 20° N with $q < 2.0 \times 10^{-5}$ K m$^{-2}$ kg$^{-1}$ s$^{-1}$) based on the ratio of DHCI/HCI. (a) January 3, 1979, nine days after the first processing event for the 1978–1979 winter. (b) January 27, 1989, just prior to the appearance of the late January 1989 minihole. (c) February 5, 1989, after the 1989 minihole (nine days after Figure 13b). (d) February 5, 1989, nine days after initialization of the special experiment when no processing is allowed before January 27, 1989. (e) February 5, 1979, same day as Figure 13c for 1979.

The results of the special minihole experiment (Exp 358) on February 5 (Figure 13d) show a smaller percentage of air processed population, but there has been an increase in both the moderately and highly processed groups.

The contour interval is 0.2 inside the vortex and 0.01 outside the vortex. The decreased interval outside vortex is to show the stretched remnants that remain after the stratospheric warming.
Processed Air Outside of Vortex, 2/5/89, Exp357

Fig. 15. Contours show potential vorticity from $2.0 \times 10^{-5}$ to $2.8 \times 10^{-5}$ K m$^2$ kg$^{-1}$ s$^{-1}$ on the 450 K surface for February 5, 1989. Large diamonds show points with highly processed air ($DHCI/HCl < 0.90$); smaller diamonds show moderately processed air ($0.90 < DHCI/HCl < 0.97$). Diamonds that cross the "edge" of vortex are due to errors in the interpolation to the 450 K surface and in the graphics routine.

with values between 0.95 and 0.99 than in the normal experiment. This could be due to the shorter duration of the experiment, so that low values are less common, but it suggests that during the minihole event in the normal experiment, previously processed air was mixed outside of the vortex, and very little processed air was formed anew outside of the vortex.

The population from the 1979 experiment on February 5 (Figure 13e) has a different character. The largest population group is 0.97-0.99, rather than 0.99-1.00, still in the slightly processed population. There are also more points in the moderately processed group 0.90-0.97, but not significantly more highly processed air with values of <0.90.

It is easy to trace this different population distribution to the minor stratospheric warming of January 1979. Even on February 5, contour maps of processed air (Figure 14) show remnants of the stretched polar vortex that formed during warming. The only region outside the vortex where values remain >0.99 are in the Aleutian anticyclone. The interior of the anticyclonic vortex is relatively isolated in the same sense that the cyclonic polar vortex is isolated. This shows that the stratospheric warming can deposit processed air outside the polar vortex. But even in this case of a severe large-scale distortion of the vortex, only air from the edge of the vortex has been effectively removed. There is no evidence of deep vortical air being deposited in middle latitudes.

The distribution of processed air outside the vortex on February 5, 1989, is more closely investigated in Figure 15. This figure is a latitude-longitude map on the 450 K surface. The contours are potential vorticity from $2.0 \times 10^{-5}$ to $2.8 \times 10^{-5}$ K m$^2$ kg$^{-1}$ s$^{-1}$, and they mark the edge of the vortex. The larger diamonds show points that contain highly processed air; the smaller diamonds are moderately processed air. Air inside the vortex is not marked.

There are two apparent features. One is the significant longitudinal variation of the processed air, as discussed by Kaye et al. [1991]. Processed air is essentially excluded from the Pacific Basin ($-120^\circ$-$200^\circ$). This is the region of the Aleutian anticyclone, and there is no obvious deposition of material south of the Aleutian anticyclone. The exclusion from the anticyclone is consistent with our earlier simulations of the satellite data [Rood et al., 1991], which showed that if large amounts of vortical air were deposited in the anticyclone, then the observed values of ozone could not be maintained. It has been speculated that the region south of the anticyclone would be an area of preferred mixing of vortical material. The two regions where processed air extends toward middle latitudes are where the vortex is preferentially distorted during winter. The presence of processed air indicates mixing that occurs during these distortions, which are related to the location of tropospheric storms.

The second feature, the general location of the highly processed air next to the vortex, could suggest localized mixing at the vortex edge. However, the possibility of numerical leakage across the edge requires consideration (see Table 2, and associated discussion). A recent numerical experiment might provide more insight into this problem. Prather's scheme was run in a fully three-dimensional (3D) experiment, in which virtually no processed air leaked across the edge of the vortex. Extra-vortex processed air was limited to small amounts in organized tongues associated with large-scale disturbances (e.g., warmings). With Prather's scheme in 3D, however, the ozone (and other) simulations degraded in quality. The character of the degradation suggested that small-scale horizontal mixing was needed. This experiment therefore suggests that the localized mixing at the edge of the vortex is not a matter of pure fantasy.

Figure 16 is different quantification of the histograms in Figure 13. This figure shows for the different days the fraction of the area in the halo around the vortex (north of $20^\circ$N, potential vorticity values < $2.0 \times 10^{-5}$ K m$^2$ kg$^{-1}$ s$^{-1}$) that is populated by air with $DHCI/HCl$ ratios less than a
The temperature at 90 is for a ratio of 0.90, and only the February 5, 1989, experiment 357 has an area much greater than about 5% that contains processed air. This increased area is due to transport by the passing minihole anticyclone.

specified value. For instance, the values at 93 show the fraction of area with ratios <0.93. The values at 90 show, that with one exception, no more than about 5% of the air in the vortex halo is highly processed. The exception is February 5, 1989, from the regular experiment (Exp 357), where approximately 15% of the vortex rim contains highly processed air. This, once again, suggests that the minihole event mixed previously processed air outside of the vortex.

**DISCUSSION**

Three general topics have been presented. The first is the documentation of the model performance in the minihole simulation. This shows the model is giving a good basic representation of transport processes. The second topic is the formation of processed air by episodic events. Combined with the results presented by Douglass et al. [1991] that show the model represents the location of processed air with some accuracy, it is concluded that the simulated episodic processing is physically meaningful. Therefore, given both the basic representation of transport processes and the relevance of the processed air simulation, the mixing of processed air out of the vortex has been examined. This mixing is the third topic. This section examines each topic in the context of real atmospheric processes.

Since the model simulates miniholes, and since there are sound physical reasons to expect miniholes with passing anticyclones, there is little doubt that miniholes exist. However, the sequence of pictures in Figure 1 does raise an interesting point. On January 30 and 31 and February 2, the model simulates the magnitude of the total ozone field with significant accuracy. However, on February 1, when the TOMS data show the most profound minimum, the model is showing the recovery of the event.

More detailed examination of the model values shows that the deepest minimum is at 0600 UT on January 31. The lowest model values are just above 200 DU. Therefore, even by 1200 UT on January 31, the time shown in Figure 1, the minihole was already in recovery. This suggests that clouds on February 1 significantly impact the TOMS measurements. There is no obvious reason to expect the assimilation to be any worse than normal on February 1, and numerical errors would not cause a discrepancy of this magnitude.

As discussed earlier, the minihole is basically a reversible dynamical event, in that chemical processes are not significantly involved. There is irreversible transport across the edge of the vortex, which includes not only the transport of material out of the vortex as emphasized in this study, but some transport of middle latitude air into the vortex. The synoptic maps show that features similar to the minihole (cyclonic scales in the troposphere) are always perturbing the lower stratosphere. Whether a dramatic minihole appears depends on the magnitude of the event, and the occurrence of the event in an area of already low ozone column in the stratosphere. The disturbances that are affecting the lower stratosphere are both cyclonic and anticyclonic. The anticyclonic disturbances are most visible, but the cyclonic disturbances also have important effects.

Heterogeneous processing caused by these events depends on the reduction of temperatures below the threshold for cloud formation. These episodic events can clearly lead to processing of significant quantities of stratospheric air. Furthermore, examination of the model begins to define a picture of the wintertime stratosphere. Prior to December, temperatures are not generally cold enough for large-scale processing to occur. Episodic events perturb the temperature to the extent that processing can occur, and through advection the vortex fills with that processed air on the time scale of a week. As January approaches, the temperatures become generally cold enough for large-scale processing. As winter ends in February and March, the episodic events once again provide a larger portion of the processing. Even during the coldest part of winter, these disturbances cause processing at the edge of the vortex, where temperatures are not as cold as in the vortex core.

The potential importance of these events is examined more fully in Figure 17. This figure shows the minimum temperature north of 32.5°N for various Decembers on the 440 K surface. These temperatures are from the National Meteorological Center (NMC) analysis and allow the temporally limited STRATAN data set to be extended to other years. The December 25, 1978, event occurs when the temperature reaches 194 K. This threshold is also clear in the 1988–1989 AASE simulations. The November temperatures for these years never show temperatures cold enough for processing at this altitude.

There is considerable interannual variability in the Decembers. Some of the Decembers (e.g., 1979, 1980, 1986) show a rapid decline in temperatures, which suggests that the atmosphere has systematically cooled and that large-scale processing is occurring. Other Decembers (e.g., 1981 and 1983) show fluctuations suggestive of disturbances of sufficient magnitude to process air in situations where processing is not otherwise possible. In either case, the data suggest that, with the exception of 1987, processed air should be present in all Decembers. Frequently, this processing occurs because a tropospheric disturbance perturbs the local temperature field below the threshold needed for polar stratospheric cloud formation. The model suggests that this early in the season, processed air remains confined to polar regions.

The temperature data at higher altitudes (i.e., 30 hPa, 600 K) show that processing occurs earlier than on the 440 K (50
The CTM runs at higher resolution and allows the important winds to produce a spectral cascade in the constituent field. This allows at least a consistent, if not realistic, representation of subscale processes. The transport algorithms are essentially nondiffusive except for the smallest resolvable spatial scales. These small scales are then only diffused when they can possibly generate unphysical maxima or minima.

While this diffusion is in fact numerical, it is not entirely unphysical. These smallest scales are diffused when their amplitude is relatively large or, equivalently, when they are about to buckle. At this point, mixing would be expected. Therefore, even though the instantaneous cascade from
buckling to mixed might not be precisely modeled, it does represent a basically physical process. The comparisons with data, as well as recent 3D experiments with Prather's [1986] scheme, suggest that the amount of mixing with van Leer's scheme at about a 2° resolution is not unrealistic.

A hierarchy of conclusions can be drawn about the chemical consequences of modeled vortex leakiness. The quantification of the amount of leakiness remains subjective. If there is a significant nonphysical numerical component, then the vortex is basically isolated from the rest of the hemisphere. If all the transport were physical, then up to 15% of the area outside the vortex (north of 20øN) might contain highly processed air. The best estimate from this model calculation is that about 5% of the extra-vortex air has been significantly processed.

The location of this processed air is a more robust conclusion. Both the 1979 and 1989 experiments show that the Aleutian anticyclone/Pacific Basin is essentially nonpolluted. Kaye et al. [1991] show preferential longitudes that these longitudes are centered at 60 and 270 E. Kaye et al. vortex systematically stretches and distorts, which is related to the presence of tropospheric storms. From Figure 15, these longitudes are centered at 60 and 270 E. Kaye et al. [1991] also show that photochemical recovery of the HCl is nearly complete by the end of March.

As for possible ozone reduction and possible chemical questions, the results address several issues. Stolarski et al. [1991] show that the trends in the TOMS data in the northern hemisphere are maximum in the Pacific and minimum over Eurasia. This is opposite of where the model would imply by direct CI destruction. Furthermore, the TOMS trends are prominent by early January, before the model shows that much significantly processed air is expected to be out of the vortex.

Toohey et al. [1991] report elevated CI0 values in early December 1989. The model, plus the analysis of December temperatures, imply that these elevated values could not come from heterogeneous processing in the vortex. The model simulations of satellite ozone and nitric acid data also show that substantial leakage of vortical air to middle latitudes in fall and winter are inconsistent with the observations. The Toohey et al. observations, the HNO3 and ozone results of Rood et al. [1990b, 1991], and the ozone trend maps of Stolarski et al. [1991], all support the notion that there are fundamental shortcomings in our understanding of middle latitude chemistry in the autumn and early winter. This could be due to heterogeneous processes on background aerosols occurring in particular light and temperature ranges; however, recent calculations by Considine et al. [1992] show inclusion of background aerosols does not provide uniform improvement of chemical model comparisons with observations.

The model confirms the existence of miniholes but also suggests that the cloud-related TOMS algorithm problems may occasionally be significant. The heterogeneous processing associated with the minihole transit can be large and produce enough processed air to perturb the CI partitioning in the entire vortex. These events are particularly important in December and late winter, or in midwinter if the winter is warm. They also process air on the edge of the vortex during the cold midwinter.

The transient disturbances transport air across the edge of the vortex. While there is transport of air both into and out of the vortex, the requirement that these events be close to the edge, coupled with the expected shrinkage of the vortex due to radiative processes [Butchart and Remsberg, 1986], imply that as the vortex shrinks during winter, there could be effectively "one way" transport. This transport would leave a residue of processed air at extra-vortex latitudes, with little associated mixing of nonvortex air into the vortex. There appears to be very little direct production of processed air outside the vortex by any of the events studied. Though it is difficult to quantify the amount of air outside the vortex that has been significantly processed, an estimate was made that 5% of the area north of 20øN and south of the vortex contained processed air. This air is not present in significant quantities until the end of January.

The extra-vortex processed air is a strong function of longitude. The ozone data suggest that direct destruction of ozone by this processed air is not the cause of the northern hemisphere ozone trend. This plus previous HNO3 model results and recent CI0 measurements support the conjecture that there are fundamental shortcomings in middle latitude low-light chemistry in fall and winter.

The model provides a picture of the evolution of the heterogeneously perturbed vortex. Processing begins at higher altitudes first (30 hPa), perhaps in late November and early December. This air remains at higher altitudes. The initial processing is correlated with episodic events that leave the processed air in the vortex both longitudinally and latitudinally structured, possibly with the most processed air forming a ring around the inner vortex. Processing starts at lower altitudes sometime during December. By January the vortex is, in general, cold enough that wholesale processing is occurring. At this time, the episodic events are important because they might force the temperatures cold enough to cause denitrification. The episodic events, which are always present, continue to form newly processed air at the edge of the vortex.

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