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Progress Report on EOS IDS

Investigation of Chemical and Dynamical Changes in the Stratosphere up to and During the EOS Observing Period

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Overview

This year's report is organized somewhat differently than last year's report in that more detailed discussion of each activity within the IDS investigation is presented. As with last year's report, there are two primary focuses of the EOS IDS investigation at this stage. The first is the analysis of UARS data. The second is the production and analysis of assimilation data by the Data Assimilation Office. Other activities, such as 2-D model development, tropospheric chemistry, TOMS trend analysis, radiative transfer work, mapping methods, and programmatic activities continue as well. These activities are described in the sections below with highlights given in this section.

There are three broad themes in the activities of this IDS. First, is assessment of dynamical processes as related to the environment for ozone changes and as related to the ability to model the atmospheric chemical process. Second is research relevant to defining EOS instrument capabilities and the production of tools to increase that capacity. Specific examples include evaluation of the EOS SOLSTICE instrument and the ongoing work with the HIRDLS instrument. Underlying all of this is evaluation of the UARS data with respect to the EOS themes. Finally, some of our activity is directly related to developing and improving assessment models, by evaluation our simulations against the UARS observations and by improving the 2D and 3D models which have been developed.

With the exception of M. Geller, none of the EOS IDS team receives money to analyze UARS data. Nonetheless this data set is the best prototype for EOS CHEM so the tools we develop and our experience from UARS data is directly applicable. A large part of our team is now focusing on the UARS data set (Schoeberl, Douglass, Jackman, Rood, Geller, and Lait) as some of that work is described in Section A below. A major result obtained under this EOS IDS is development of a model for the recovery of the ozone hole - that is the re partitioning of radical chlorine into reservoir species at the end of winter. We feel that this work, which involved a group of UARS instruments is a major breakthrough.

About 1/3 of this EOS IDS money goes to the Data Assimilation Office (DAO) for production of the Stratospheric Analysis. The money being sent to the DAO supports preparation the data and production runs of the model. A lot of progress has been made on the stratospheric assimilation side as reported below. This includes UARS temperature assimilations and preliminary work on constituent assimilation. We received an augmentation to the IDS investigation late last fiscal year which helped us begin the constituent assimilation work. Since the augmentation arrived late in FY94, part was used to upgrade hardware and forward fund existing investigators then the EOSDIS money for next year will be used (partially) for personnel costs. We also began the interview process for two hires - one individual to be dedicated to the stratospheric analysis and a second to lead the chemical assimilation effort. We will also use the augmentation to develop the forward model for the assimilation of chemical species. This model will be developed by GATS Inc. for assimilating the CLAES N2O. Details of the assimilation effort are described in Section B.

During the last reviews, we discussed the MODE (Multi-year Ozone Depletion Experiment). That experiment is intended to perform an analysis of each year on the NMC data and to crudely simulate the ozone loss using heuristic relationships derived from the AASE II aircraft data. We are now setting the stage to begin the experiment All of the NMC data sets have been analyzed for NAT formation temperatures and persistence of PSC's. After a considerable effort trying to get the optical Jukeboxes to work with our workstation we have used the EOSDIS money to purchase several 10 gigabyte hard disk drives. All of the NMC analysis, 1979 - 1994 has been transferred to these disks (a considerable effort). We will also be transferring this data to the GSFC DAAC within the next year as part of our EOS activity. We are also in the processing of transferring all of the UARS chemical and meteorological data to the 10 gigabyte drives.

Descent within the vortex has been clearly demonstrated by the UARS HALOE data. This descent complicates the MODE experiment since the air processed within the vortex will have descended from higher altitudes and thus have different total Clx than air sampled at 440K during September. To understand the effects of this descent, we have first checked that it is consistent with the RT models used within the group. This has been done, and the results have been published (Rosenfield et al, 1994). We have also performed an extensive analysis of the HALOE data to determine the rate and magnitude of the descent. This was done to check the analysis of Russell, Tuck and co-authors who claimed that descent rates were 7km/month. Our analysis, (Schoeberl et al., 1994), shows that the Russell-Tuck analysis to badly flawed and that descent rates we compute from the same data are consistent with radiative transfer models.

Last year we performed a prototype MODE calculation on a swarm of parcels within the vortex. The trajectory chemistry model was then run on the descending particles to determine ozone loss. The cost of the calculation was prohibitive. It became clear that we would need to develop a quick and dirty trajectory chemistry model to complete the 15 year study. Section I below discusses that status of that part of the project.

Wholly under this IDS, the interactive 2D model is being developed. The dynamics of this model were submitted for publication last year and are in press (Bacmeister et al., 1994). This year we hired a person to work on the model full time: this effort included coupling the chemistry and dynamics, tuning the tropospheric circulation, and beginning the Pinatubo test problem. The short term research goal of this effort is to determine why the ozone loss associated with the Pinatubo eruption appeared the second year after the eruption, not the first. To do this we have developed an aerosol climatology and are using that along with the radiative transfer code to force the model. Section C describes this and other work in the 2D modeling area. Preliminary results suggest that the dynamics of aerosol heating created an anomalous circulation the first year which masked chemical ozone loss. This circulation died down the second year so chemical loss became more apparent.

In tropospheric chemistry we have focused mostly on development of better methods for satellite retrieval of tropospheric ozone. In addition, some modeling of gases related to tropospheric O3 change (CH4, CO and NOx) continues at a modest level. This effort is described further in Section E.

Under this IDS we also continue to perform TOMS data analysis. Although this effort is small, it is not duplicated within the other TOMS activities. Results of the real-time analysis of Antarctic ozone depletion in 1994 were used in the GSFC October press release. Section F details this effort.

Using the trajectory model we are now able to compare different trace gas data sets using trajectory mapping technique (Morris et al., 1994). Trajectories are initiated whenever the instrument makes measurements. Then when the trajectories pass near each other. The data can be indirectly compared. This system has been applied to the UARS data comparing ozone, water and N2O from different UARS sensors. A new and more powerful variant of trajectory mapping has been developed - it is called time-space threading and promises to be able to make very precise high resolution maps of constituent data from parcel trajectories. Efforts in this area are discussed in Section G.

At Stony Brook, our CoI is beginning an effort to look at the sampling strategy for the EOS HIRDLS instrument. Using a high resolution transport model, we are moving a tracer around then re sampling the tracer with the HIRDLS scan pattern. This should give us exact insight into the capabilities of the HIRDLS instrument. This effort is described in Section H.

Finally, this IDS has performed a number of programmatic duties associated with the EOS effort at GSFC. First, the PI, Dr. Schoeberl, also held the extra duty of the CHEM Project Scientist for most of FY 1994. Dr. Gleason, was added to the IDS team in 1994 and he became the CHEM Project Scientist in August, 1994. Two major EOS activities occurred during the summer. First, we were heavily involved in the EOS restructuring which took place in June and culminated with the Payload Panel meeting in July. Through our efforts, the CHEM mission was not slipped from its 2002 launch date and SOLSTICE and ACRIM were not dumped from the payload. Second, we sponsored a workshop in early July to get the community to endorse the measurements on CHEM. They did so, and that workshop report will be shortly published in the Earth Observer.

EOS IDS Budget

Long ago, the original EOS IDS Budget assumed that constituent and stratospheric data assimilation would be performed by this IDS team. Under the revision of the proposal, it was decided to move our assimilation to the Data Assimilation Office DAO. The DAO would do the stratospheric assimilation, and our IDS effort would provide funding augmentation for preparation of the data, quality control and constituent assimilation. Steve Cohn was added as a Co I to provide expertise in the area of constituent assimilation.

As can be seen from the budget for last year, two new assimilation tasks have been added. Next year, Dixon Butler has informed me that the augmentation will come through EOSDIS directly to the DAO. Thus these temporary tasks (Assimilation 3 and 4) will be transferred to the DAO budget. The projected 1995 budget is indicated with $20K shortfall. This shortfall will be absorbed in hardware purchase form EOSDIS money.

A. UARS Data Analysis

The Microwave Limb Sounder observations of ClO provide global information about heterogeneous reactions on the surfaces of polar stratospheric clouds (PSC's) through which ClO is released from the reservoir gases HCl and ClONO2 in the lower stratosphere. In early December 1991, high values (> 0.5 ppbv) of ClO are seen sporadically by MLS within sunlit regions of the north polar vortex. In no case are the observed values coincident with temperatures cold enough to support polar stratospheric cloud formation.

Douglass et al. (1993) report the results of a three-dimensional simulation for December 1991. The wind and temperature fields used in this simulation are taken from the Goddard Data Assimilation procedure, thus the results of the simulation may be compared directly with the observations. A simple parameterization for HCl photochemistry based on the Goddard two-dimensional model is used for this calculation. Two simulations are performed. In the first, HCl is calculated using transport and the parameterized photochemical production and loss. In the second simulation, HCl loss is increased when the temperatures are colder than a critical value. The difference between these two simulations, DELTA, is a marker of air in which heterogeneous reactions have taken place. This air is expected to have elevated ClO when sunlit.

The results of the simulation are shown in the sequence given in Figure A1. The thick contours are area where the temperature is cold enough for PSC formation. The x's show the sunlit portions of UARS flight track for each day. The contours of DELTA (thin lines) are advected away from the cold temperatures, and occasionally reach lower latitudes where they could be sunlit and observed by MLS. The MLS observations for the same days are shown in Figure A2. Some of the features shown in these maps are near the noise level of the instrument (0.5 ppbv), and are not significant. Several of the features show remarkable similarity to the calculation. A feature which is apparent on Dec. 7 intensifies on Dec. 8, and then weakens on Dec. 9, similar to the simulation. On December 10, the highest values of DELTA have moved poleward, and MLS sees no elevated values. A new region of high values appears on December 11, which intensifies on Dec. 12-13. The most intense feature seen by MLS on December 14 is only seen weakly in the model, however, suggesting that the temperatures in the model are not as cold as in the atmosphere.

The model also shows that the magnitude of DELTA decreases following an event as a result of transport and mixing, indicating the importance of a good analysis of the dynamical effects when trying to derive chemical information from observations. This concept is also shown in the work of Schoeberl et al. (1993a). Analysis of the UARS MLS observations in early January 1992 shows a clear relationship between predicted polar stratospheric cloud formation along back trajectories and elevated ClO amounts. These finding were shown to be in good agreement with previous analysis of aircraft observations (Schoeberl et al., 1993b). The decrease in ClO following the PSC encounter was found to agree well with the decrease calculated using a photochemical model when the trajectory of the parcel, which determines the amount of insolation, is accounted for. This work also showed that the occasional high values of ClO seen by MLS outside the polar vortex are accounted for by a statistical analysis of the distribution of MLS values.

One advantage of the UARS data set is that many of the key stratospheric constituents are observed by at least one of the instruments. It is possible to combine observations from different instruments by accounting for dynamical variability. This is demonstrated by an analysis of Cryogenic Limb Array Etalon Spectrometer (CLAES)observations of ClONO2 and HNO3, Halogen Occultation Experiment (HALOE) observations of O3, HCl, NO and NO2, and MLS observations of O3 and ClO recently submitted by Douglass et al. (1994).

Maps of ClO, ClONO2, HNO3 and O3 for the northern and southern hemispheres show the major differences which lead to the formation of the ozone hole. In the southern hemisphere, deep within the polar vortex, the HNO3 is removed from the stratosphere. ClO levels are high, ClONO2 values are low, and O3 depletion is drastic. Nearer to the vortex edge, temperatures are still cold enough to produce nitric acid trihydrate (nat) PSC's, but not cold enough for ice clouds. Here both HNO3 values and ClONO2 values are large, forming a "collar" surrounding the inner vortex. ClO, while elevated, is much lower than deep within the vortex.

In the northern hemisphere, low values of HNO3 are found only when nat PSC's are actually present. High values of ClONO2 are seen at the end of the winter, and moderate O3 values. It was thought that the photochemistry of the northern hemisphere would resemble the photochemistry of the "collar" region.

Time series of O3, ClO, ClONO2, HNO3, NO, NO2, HCl and temperature are produced by averaging the observations using surfaces of constant potential temperature (constant entropy) for the vertical coordinate and modified potential vorticity for the horizontal coordinate. The results are shown in figures A-3 and A-4 for the northern and southern hemisphere. There are surprising differences.

In the northern hemisphere, ClO is low, ClONO2 is high. HNO3 is high. There is little evidence for loss of O3. The NO seen by HALOE is significantly lower than the NO2; HCl shows a slow rise as expected as the chlorine reservoirs seek their normal balance. Throughout most of the spring, ClONO2 is the principal chlorine reservoir.

In the southern hemisphere collar, ClO is elevated throughout the UARS southern yaw period, producing steady loss of O3. The ClONO2 does not rise, however, in spite of the sunlight and the high values of HNO3. When the O3 falls below about 0.5 ppmv, the HCl starts to rise rapidly. Also during this time period, NO rises rapidly. These observations allow identification of the chemical mechanism which is responsible. When O3 falls to low values, the reaction to produce ClO (Cl + O3) and to produce NO2 (NO + O3) both become less important. The concentration of Cl rises because the loss of Cl is reduced (Cl + O3). Furthermore, the production of Cl is increased (NO + ClO) because the loss of NO is decreased (NO + O3). Thus production of HCl through Cl + CH4 rises non-linearly. HCl becomes the dominant reservoir for chlorine in the southern hemisphere spring due to low O3.

B. Stratospheric Data Assimilation

The stratospheric assimilation effort has focused on two activities, traditional meteorological assimilation and prototype constituent assimilation. The meteorological assimilations have been performed with both a research version of the Goddard Earth Observing System (GEOS), Data Assimilation System and the stratospheric configuration of GEOS, STRATAN.

Accomplishments in the stratospheric assimilation include:

1. A two and one half year UARS assimilation

2. Operational support of the ASHOE MAESA campaign

3. Use of the assimilation in successful 3-D transport chemistry applications

4. The assimilation of UARS temperature observations

5. Improvements of the polar numerics in the assimilating models.

6. A theoretical study of the impact of the HIRDLS scanning

7. Development of the components for Kalman filter constituent assimilation

8. The use of STRATAN winds in chemical assessments.

B1 Meteorological Assimilation

The highlights have been the production of a two and a half year data set that started at the time of the launch of the Upper Atmosphere Research Satellite (UARS) and operational support of the ASHOE/MAESA aircraft campaign. The UARS period assimilation has been used in the three-dimensional stratospheric chemistry model (A. Douglass, PI). A notable accomplishment is a one year integration of ozone using parameterized chemistry. As shown in Figure F1, in the middle latitudes of both hemispheres the assimilation winds are capable of representing the observed total ozone variability with significant accuracy. In the subtropics and tropics the variability in the chemistry model is higher than in the TOMS observation. At the equator a bias develops, but it is self limiting and is due to ozone loss in the troposphere. This suggests that the previous bias caused by the excessive upward branch of the Hadley circulation (Weaver et al., 1993) has been corrected. A second application in the 3-D chemistry effort has used the full chemistry model. This application has shown that the assimilation winds represent dynamical variability with sufficient accuracy to allow direct quantitative comparison with the UARS data. In addition, the fact that the model/UARS correlations are maintained on seasonal time scales increases the confidence that the chemistry transport model provides an accurate representation of the atmosphere during the period that the UARS instrument is not observing poleward of 34 degrees latitude.

The operational support of the ASHOE/MAESA mission provides forecasts for flight planning and assimilation analyses to aid in the interpretation of the constituent observations. For flight planning, the forecasts are used with contour advection models to predict high resolution features in the constituent fields. R. A. Plumb has reported that the winds from the GEOS assimilation have provided superior forecasts of constituent variability. In addition, P. Newman et al. have been able to use the assimilation to provide quantitative interpretation of heterogeneous chemical processing.

These applications to chemistry and transport problems provide stringent tests of the assimilation and direct attention to shortcomings that need improvement. Two problems which appear common to all stratospheric meteorological analyses are a warm bias at polar latitudes during extremely cold periods and poor representation of instantaneous winds in the tropics. In addition, the studies have revealed two persistent, possibly related, polar problems in the GEOS system that are probably artifacts of the data assimilation system.

These two polar problems are excessive noise at the pole, especially when there is cross-polar flow, and a persistent upward signal in the residual circulation at the South Pole. The polar problems could be related to the assimilation system or some more subtle conceptual error in the formulations of the system. If an artifact of the assimilation system, then the problem could be related to the assimilating model or the analysis routine.

Attention is currently on the assimilating model (see Takacs et al., 1994). Figure F2 shows a characteristic example of the polar noise problem and the same experiment with a research version of the GEOS model. The polar noise is absent from the research version of the model. These results were achieved by rotating the computational pole to the equator. Numerical problems at the equatorial computational pole are not apparent and may be related to the fact that the Coriolis term is small at the equator. Near term plans call for experiments to see if the polar rotation impacts the problem with the residual circulation.

The warm bias at cold polar temperatures is very likely related to data problems, combined with a tendency for the model to underestimate the most extreme events. A recent experiment using UARS temperature data in the assimilation shows promising changes in the assimilated data products. Figure F3 shows a comparison of winds from an assimilation that uses UARS data and one that does not, with the highly accurate wind measurements from the ER-2 aircraft. This case was the worst case comparison of the conventional assimilation during ASHOE/MAESA.

Despite the short comings discussed here, the transport experiments with the assimilation demonstrate state-of-the-art results. A time series of winds (Fig. F4) reveals a credible representation of the quasi-biennial oscillation. Because of these superior characteristics winds from the STRATAN assimilation will be used in 3-D assessments of the impact of stratospheric aircraft. This represents an important contribution of the EOS effort to the quest to assess environmental change.

Short-term plans call for a series of experiments to improve the transport characteristics of the assimilation winds. These include assimilation experiments with the rotated pole version of the Eulerian GEOS model as well as with the semi-Lagrangian dynamical core. These experiments are expected to improve the short time scale polar flow as well as characteristics of the residual circulation. Improvement of tropical dynamics represents a more difficult long-term problem which may defy substantial improvement until more complete input data sets are available. B2 Stratospheric Constituent Assimilation Constituent assimilation has a special role in the assimilation effort. It not only provides a scientifically useful product, but provides an effective mechanism to build advanced assimilation capabilities. The role of constituent assimilation, plans, and interactions with NMC are described in the Data Assimilation Office Plan. The Strategy Statement on Constituent Assimilation from that plan is attached as an appendix.

Initial experiments with an idealized model have focused on the impact of the scanning capabilities of HIRDLS, compared with the single profile limb view of the UARS instruments. First results show that the scanning capability of HIRDLS does allow effective filling in of the tracer spectra. In addition, there is evidence that assimilations can fill in large unobserved regions such as the ones present in the UARS viewing geometry.

A milestone targeted for early 1995 is the assimilation of UARS N2O on isentropic surfaces. A series of surfaces have been chosen to cover the lower and middle stratosphere, 450-800 K. These surfaces cross a region that contains both synoptic and planetary scale dynamics at lower altitudes to a nearly pure planetary scale regime in the middle stratosphere. Winds will be derived from the STRATAN assimilation system. They will drive a Kalman Filter assimilation system based on the advection model of Lin and Rood (1994). This will be the first realistic application of a Kalman Filter assimilation system in Earth science.

Currently the Kalman filter is running on the massively parallel Intel Delta computer. The interface with the STRATAN winds has been accomplished. Presently the UARS N2O observations are being prepared for input. This includes defining the N2O error characteristics.

C. Interactive two dimensional model

The 2D interactive model is starting to come to maturity. Simulations of column ozone and other constituents are fairly reasonable when compared to measurements Figure C1 shows some of the preliminary results from the model. As mentioned above, work is proceeding on the chemical model and inclusion of aerosols for the Mt. Pinatubo experiment. During the last summer, a preliminary version of a QBO forcing system was installed in the interactive 2-D model, but this need considerable more tuning. The model also requires more attention on the troposphere and tuning the gravity wave representation. However, with a full time person working on the model, the pace of improvement has increased significantly. We believe that within the next fiscal year, the model will yield several important papers for publication..

The work on solar proton events (SPEs) is also related to the EOS IDS research. We have tried to simulate the effects of the very large SPEs of October 1989 with both our 2D and 3D model. In Jackman et al. 1993, 1994) we noted the importance of properly representing the polar vortices and warming events and the importance of the interannual variations in the downward transport when studying the atmospheric effects of the SPEs weeks to months after the events. We also showed that our simulations of the NOx increases during the SPEs are very close to observations and that these large SPEs can have a significant impact on polar lower stratospheric NOx a few months after the events.

D. Radiative transfer work

Heating rates computed with a radiation model and NMC temperature observations were used in a one-dimensional vortex interior descent model to determine diabatic descent rates for the fall and winter periods in the northern hemisphere for 1988-89 and 1991-92, and in the southern hemisphere for 1987 and 1992 [Rosenfield et al., 1994]. The computed descent rates generally agree well with observations of long-lived tracers [Rosenfield et al., 1994; Strahan et al., 1994], thus validating the radiative model. These results argue against the "flowing processor" concept of the polar vortex, which would require much larger cooling rates than those computed.

Several molecules important in the chemistry of the stratosphere photodissociate in the Schumann-Runge bands of oxygen, a spectral region in which the penetration of solar radiation into the middle atmosphere varies by several orders of magnitude as a function of wavelength. It has been suggested that a knowledge of the fine structure of the solar spectrum is thus necessary for an accurate calculation of photolysis rates for these molecules. If this information is required then extremely precise knowledge of the UV solar spectrum is needed. Such precision is available with the SURE option on EOS SOLSTICE. Computations of the sensitivity of the computed photolysis rates to the solar spectral resolution show that knowledge of the fine structure in the Schumann-Runge region of the solar spectrum produces only a marginal (1 -2 %) improvement in the computation of photolysis rates [Rosenfield, 1994]. As a result of these calculations, the SURE option was deselected saving the program several million dollars. The evaluation of the SURE option was made by this IDS investigation.

Work has been ongoing on studying the radiative and dynamical effects of the Pinatubo volcanic aerosol. A parameterization of the optical thicknesses of both the background and the volcanic aerosol has been developed for use in our wide band radiative transfer model. SAGE II observations of 1 micron extinctions, along with Mie calculations of absorption and extinction cross sections using observed particle size distributions for the sulfate aerosol, have been used. Fig. D1 shows the computed perturbation to the net heating for November, 1991. The distribution of more heating in the tropics and more cooling in the high latitudes would lead to a change in the diabatic circulation giving more upwelling in the low latitudes, and more downwelling in the high latitudes. This parameterization has been incorporated into our two-dimensional interactive radiation/dynamics/chemistry model and we are studying the radiative/dynamical effects of the aerosol on ozone and other stratospheric species.

E. Tropospheric Chemistry Studies

Two major activities in this area are (1) using models to evaluate the role of convection in stratospheric-tropospheric exchange and O3 formation (co-funded with Tropospheric Chemistry and ACMAP [Atmospheric Chemistry Modeling and Analysis Program]); (2) development of tropospheric O3 satellite products (co-sponsored with ACMAP, and in FY95, with UARS). Considerable progress in each area was made in FY94. In the convection- chemistry area, we published a regional estimate for the deep convective CO flux in the summertime midwest US [Thompson et al, 1994] and compared the convective flux for the same region obtained by the GCEM (Goddard Cumulus Ensemble Model) and GEOS-1 [Pickering et al, 1994; see Figure E1].

A major study of CO flux with the GCEM and MM5 mesoscale model is being conducted for a TRACE-A case study (Flight on 27 Sept. 1992) - it appears that significant O3 formation took place in cloud outflow layers and could be observed in soundings hundreds of km downwind. We are performing photochemical model calculations of TRACE-A data in conjunction with the tracer studies. In the category of remote sensing, research on retrieving tropospheric ozone from TOMS (in the tropics) has produced one paper in press [Hudson et al, 1994] and another is about to be submitted [Kim et al, 1994; See Figure E2]. Time-averaged, high-density maps for an initial study period (6-21 October 1992, coincident with the TRACE-A and SAFARI field missions) showed excellent agreement with soundings. These maps are suitable for modeling analysis [Thompson et al, SAFARI Book Chapter, in preparation, 1994]. Methods for daily maps are still being perfected. In the process of validation of the tropospheric ozone maps, we have assembled a climatology of tropical soundings that will feed into future TOMS, UARS and EOS investigations.

F. TOMS Data Analysis

Aside from UARS data, this IDS spends some time looking at TOMS data and performing analysis of global ozone amounts. A TOMS-like instrument will be launched on EOS CHEM and simulations of ozone change have to fit within the TOMS observational set. We are currently continuing our analysis of the ozone hole data. Figure F1 shows the size of the ozone hole averaged between mid-September and mid-October. The size is basically the area enclosed within the 220 DU contour. Preliminary 1994 data show that the size is comparable to that in the previous three years. The ozone hole size appears to have stabilized to a fraction of the vortex area as predicted by Schoeberl and Hartmann (1990).

Critics of the anthropogenic chlorine theory for south polar ozone loss frequently point to the ozone hole of 1958 as proof that the ozone hole is natural. Newman (1994) has shown that the Dumont D'urville data showing the 1958 ozone hole is deficient. It neither checks with data from near by bases, nor is it self consistent. This work, supported by this IDS, closes an argument by regulatory critics. Another argument we are near closing is that volcanic chlorine is causing the ozone depletion. Evaluation of UARS HCl and HF data are underway to show that most of chlorine is due to photolysis of chlorofluorocarbons.

G. Trajectory Mapping Methods

The trajectory mapping technique was developed under this IDS and has been accepted for publication in JGR (Morris et al., 1995). The basic method is to initialize a parcel at each measurement time for some instrument then carry the parcel forward in time using a trajectory model. The method makes maximal use of the data over a short period of time and compares favorably with Kalman and Salby-Fourier methods. The additional advantage of trajectory mapping is that missing data can be easily handled and the maps can be made at any synoptic time. Using trajectory mapping, we have been examining the systematic differences in instrument measurements. Figure G1 shows comparisons between SBUV2, MLS, CLAES and HALOE data.

The trajectory mapping technique also allows us to bring together non coincident measurements such as those made by HALOE, MLS and CLAES. We have been able to use this information to work out the chlorine budget in the stratosphere (Dessler et al., 1995, to be submitted).

One of the problems with trajectory mapping has been the inability of the method to form a regular grid at synoptic times. A new method of organizing the trajectories developed by Sutton et al. (1994) generates a regular grid from the trajectories. Applying a variant of Sutton's technique, which we refer to as Reverse Domain Filling (RDF), we are able to add a high level of precision to the regularly gridded map. Figure G2 shows an example of the power of this new technique. N2O maps from ISAMS are generated using the new technique, space-time threading, and the asynoptically gathered data for one day. The dramatic improvement in the picture of the trace gas fields will have a significant impact on the sampling strategy used for HIRDLS. It will also have a dramatic impact on transport modeling since trajectory mapping provides a cost effective nondiffusive transport scheme for comparison to 3D models.

H. HIRDLS Simulation Studies

The objectives of HIRDLS on EOS are to make horizontal and vertical observations at higher resolutions than have been previously made, and also to observe the upper troposphere and lower stratosphere with improved sensitivity and accuracy. This goal is slightly different from the assimilation impact studies indicated above in that we are trying to determine what improvement to the sampling strategy can be obtained.

Investigation is being made into the "value added" by HIRDLS by virtue of the azimuthal scanning capability of HIRDLS relative to the previous observations by limb viewing instruments that scanned only in elevation (e. g., LIMS, ISAMS, CLAES, MLS, etc.). We do this by sampling model output using the anticipated HIRDLS sampling pattern and comparing the derived picture obtained with and without the HIRDLS azimuthal scanning. The first simulations of HIRDLS measurements will be made using the Goddard STRATAN and 3-D Chemical-Transport Model (CTM) results. The CTM results used will be with 2 (latitude) by 2.5 (longitude) degree resolution. We will study the sampling of both the dynamics (from STRATAN) and constituent (from the CTM) fields.

Anticipating that the constituent field should show more variability at small scales than the dynamics variables, we are also going to do similar HIRDLS sampling using a higher resolution model. This model is being constructed using the STRATAN dynamics mapped onto an isentropic surface. Then, a 2-D CTM will be run starting from an initial CTM field. In this run, the tracer will be assumed conservative. This model will be run at much finer horizontal resolution than the 3-D CTM. In this way, we will check on how much the results of the simulated HIRDLS sampling study depends on model resolution.

This work was begun last summer as an M. S. thesis investigation of Ms. Jyoteka Virmani). Thus far, we have developed a model of the observational track, without elevation or azimuthal scanning. We are implementing these scanning patterns now. Also, a 2-D transport code (developed at GSFC) has been brought over to a Stony Brook workstation and has been tested on that platform. The interpolation scheme to put STRATAN and/or CTM fields on isentropic surfaces has been developed. Our goal is to have this thesis investigation completed in about 9 months or so that we may better understand the advantages of HIRDLS sampling compared to previous limb scanners.

I. MODE Project

The overall goal of MODE (Multiyear Ozone Depletion Experiment) is to bring together diverse data sets to attempt to define the cause(s) of the observed long-term change in ozone within the vortex (see Fig. F2).

To work on this problem we have begun a series of studies using a box chemistry model integrated along calculated air parcel trajectories which end on measured data points. The measurements considered thus far are those from UARS and the polar aircraft campaigns (Schoeberl, et al., 1993; Schoeberl et al., 1994; Douglass, et al., 1994). These studies reveal that the instances of high measured concentrations of ClO can be traced back to air which has been exposed to temperatures cold enough to form PSC's. Furthermore, the ClO concentrations can be shown to be consistent with a dependence on the amount of solar exposure to which the parcel has been subjected. This dependence on solar exposure is consistent with model calculations of the expected dependence. These trajectory studies are anecdotal and show that we understand some of the important aspects of the chemistry of polar air parcels as they are spun off to midlatitudes during vortex disturbances. .

To attack the problem from a chemistry on trajectory viewpoint, a simple parametric chemical model is being developed to be run on many thousands of trajectories to obtain statistics of the potential effect of polar processes and ozone loss. Results can then be compared to runs of the 3D CTM to check for consistency. The eventual goal of this study is to be able to show whether or not polar processing followed by advection of filaments to lower latitudes explains the observed trend in ozone. A further check on will result from determination of whether such effects can explain aspects of the observed interannual variability. The continuing polar aircraft missions and the multi-year global data sets obtained from UARS should give us some critical tests of these ideas.

I1 Calculation of chemical ozone loss for northern winter

Gloria Manney (UARS Science Team Meeting, Nov. 1994) presented a trajectory analysis of the chemical ozone depletion for the northern winters of 1992-3 and 1993-4. She initialized a large number of air parcels with measured values of ozone from MLS. She then did forward trajectory calculations for about 30 days (mid February to mid March) assuming that ozone is a passive tracer. These results were then compared to actual ozone measurements and the difference identified as "chemical depletion of ozone". A more difficult question which needs to be asked is what part of this chemical depletion is due to the enhanced chlorine concentrations from fluorocarbons and what part would have occurred anyway.

We can use the trajectory chemistry code to attempt to answer this question. The trajectory chemistry code has been modified by Gary Morris to include the photolysis lookup table derived for the 3D CTM by Randy Kawa. The major problem with doing such a calculation is how to initialize the chlorine and nitrogen partitioning for the parcels. Possibilities include:

1) Use CLAES chlorine nitrate and nitric acid, HALOE HCl and nitric oxide mapped like Gary did in his thesis,

2) Map parcels back to when they last saw temperatures below the NAT saturation level and assume complete processing at that point,

3) Assume that at the start the vortex is completely filled with processed air at a specific time and everything outside the vortex has "normal" chemistry.

We can then release a large number of parcels and run the chemistry forward in time to calculate the chemical component of the ozone depletion. If this reproduces the observed changes then we can say that we understand the chemical component. If this is so, then the chemical trajectory calculations could be rerun with background chlorine (or anything in between) to determine the magnitude of the excess ozone depletion due to chlorine from fluorocarbons.

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Figure Captions

Figure A1 Model contours of Delta (ppbv) at 50 hPa for the northern hemisphere December 7-15, 1991. The bold contour is the region where the temperature T is cold enough for formation of polar stratospheric clouds. The x's indicate the locations of sunlit measurements.

Figure A2 MLS observations of ClO (ppbv) in the northern hemisphere at 46 hPa for December 7-15, 1991. The contours are 0.7 + 0.1 N ppbv.

Figure A3 Southern hemisphere time series for observations from MLS (O3, ClO), CLAES (HNO3, ClONO2) and HALOE (O3, HCl, NO, NO2) binned by MPV. The bottom panel contains the time series in the average and minimum latitude of the observations, as well as for the average temperatures (taken from NMC) for the points within the MPV band.

Figure A4 Same as A3 but for the northern hemisphere.

Figure B1 Total ozone time series at specified locations. The dashed line is total ozone from the TOMS instrument. The dark line is from the 3D transport and chemistry model. In this experiment winds from the STRATAN assimilation are used to transport the model ozone. A simple chemistry parameterization is used to provide the production and loss terms.

Figure B2 Ertel's potential vorticity on the 840 K isentropic surface. This figure shows the impact of rotating the computational pole to low latitudes to reduce spurious noise generated by numerical artifacts. The left panel shows noise at the pole and the right panel shows the contours extending across the pole in a more physically meaningful pattern. Moving the computational pole to low latitudes does not have obvious deleterious effects on the low latitude simulation, possibly because of the smaller Coriolis force.

Figure B3 GEOS assimilation minus the zonal wind measured by the ER-2. The NOUARS curve shows the standard data product derived with all satellite data coming from TOVS. The UARS curve shows the impact of the MLS temperature observations on the assimilation. The bias between the assimilation and the aircraft observed winds are reduced substantially. The aircraft flies at approximately 50 mb, and the MLS data are used at 22 mb and above. The MLS data are, therefore, impacting the analysis at lower altitudes. This influence does not extend into the aircraft dive as indicated by the overlapping curves. The MLS assimilation also locates the vortex edge closer to that indicated by the aircraft N2O observations.

Figure B4 Time series of equatorial zonal mean winds. The alternating easterlies and westerlies indicate the QBO. The left panel shows the STRATAN product and the right panel shows the assimilated product from the United Kingdom Meteorological Office. Note that the semiannual oscillation at high altitudes has less amplitude in STRATAN.

Figure C1 Top graph illustrates the total ozone (in Dobson Units) as a function of time (in months) and latitude computed with the GSFC coupled 2-D model. Bottom graph shows total ozone computed by the TOMS instrument for comparison purposes.

Figure D1 shows the computed perturbation to the net heating for November, 1991.

Figure E1. Mass flux of carbon monoxide from boundary layer to free troposphere for June 1985 over the central United States. (a) computed from GEOS-1; (b) based on statistical/dynamical method using GCE transport statistics and ISCCP cloud cover data. Lower limit estimates given by shading and upper limit estimates are contoured. (From Pickering et al, GRL, submitted, 1994).

Figure E2. Time-averaged tropospheric O3 column for 6-21 Oct. 1992 by University of Maryland-GSFC revised method (from Kim et al, JGR, submitted, 10/94). Contours are in 3 DU intervals.

Figure F1 Ozone hole area as a function of year derived from the TOMS data.

Figure F2 Data from Newman.

Figure G1 Comparison of trace gas measurements using trajectory mapping.

Figure G2. Asynoptic map of ISAMS N2O data for January 12, 1992 at 100K, (part a). Reconstruction of the field using time-space threading. Note the dramatic increase in detail.

Figure H Sampling pattern for non scanning limb sounder (part a) verses the sampling pattern for a scanning limb sounder like HIRDLS (part b).

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