CHAPTER 2

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REPORT ON THE 2-D MODEL

INTERCOMPARISON WORKSHOP

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Section 2.1 Introduction

In our attempts to understand the processes which affect ozone in the stratosphere, and to predict future ozone levels, atmospheric scientists have developed and employed a variety of computer models. To oversimplify somewhat, they range from 1-D models with intricately detailed photochemistry but only the crudest representation of transport, to 3-D general circulation models with intricately detailed dynamics and no photochemistry at all. Each of these has its appropriate uses. Many investigators have felt that there was much to be gained from intermediate models incorporating an extensive treatment of photochemistry within a dynamical framework which at least recognizes that atmospheric motions are advective as well as diffusive, and that both chemistry and dynamics are subject to latitudinal and seasonal variations. Thus the 2-D, zonally averaged models have begun to play a larger role in the last several years, both in attempting to understand observed distributions of trace species and in attempting to assess the probable effects of anthropogenic perturbations.

There are many choices to be made in developing a model, from the basic transport representation to the sources of the required input data; it would be most surprising if all investigators made the same ones. It was the purpose of the 2-D model Intercomparison Workshop to permit many investigators to discuss the choices made and the behavior of the resulting models. Our goal was not to identify a best set of choices, but rather to identify areas in which the models are sensitive to the choices made, and to develop a sense of where these models as a class do well or poorly in simulating the observed atmosphere. The discussion in this report will be quite general. However, as described in Section 2.8, a database of model output fields has been established at NASA/Langley Research Center. Readers interested in specific results are encouraged to obtain them from the database as outlined in Section 2.8.

Section 2.2 Description of 2-D Models

The basic structure of the models presented at this workshop is that of a grid point model in which each cell represents an average of conditions around a latitude circle. Transport between cells is by both advection and eddy diffusion, the details of which vary among models. Chemistry is treated as a local process in which the reaction rates depend on the temperature and solar rates during a day-night cycle in different ways. The time evolution of the concentrations of different molecular species is then followed by integrating the species continuity equations. The method of integration and the temporal resolution vary among models.

Early formulations of 2-D models expressed atmospheric transport processes in terms of prescribed zonal mean circulations and Fickian eddy diffusion (Prabakhara, 1963). The advection and eddy diffusion were treated as independent processes whose local values (wind velocities and diffusion coefficients) could be determined by observation of atmospheric motions and tracer distributions. Following the development of Lagrangian mean theory (Andrews and McIntyre, 1978) it became clear that the transports due to zonal mean and eddy motions should nearly cancel, and that the classical Eulerian framework used in early models placed severe demands on the accuracy of the calculation of the small residual from the combined transport effects.

More recent 2-D model transport formulations have been developed to be consistent with Lagrangian mean theory by incorporating the near cancellation of the zonal mean and eddy contributions and relating the residual transport directly to external forcing (i.e. diabatic heating and zonal momentum forcing). Perhaps the most widely employed such formulation at this time is the Residual Mean Circulation (RMC) form (WMO, 1986). As will be discussed below, however, this exchanges one data problem for another, since neither heating nor momentum forcing is directly observable. Both must be derived from temperature measurements and are highly sensitive to errors therein.

Another area in which the models differ greatly is the time scale at which various physical processes are resolved. For example, it is not clear a priori that photolysis rates must be recalculated for each

time step in the temporal integration. Because the computation of photolysis rates is relatively time consuming, it is tempting to recompute them only "as often as necessary" - an interval which is in practice determined subjectively by each investigator for the specific simulation at hand. The effects of the choice of this interval on the results of long integrations are still not well understood and the intervals chosen by different investigators span a wide range. Different numerical approaches also lead to varying degrees of model variability and sensitivity to uncertainties in input data.

Section 2.3 Sensitivity of 2-D Models

In previous intercomparisons of 1-D photochemical models the procedure adopted was to standardize the inputs to the participating models and compare the outputs, which in 1-D are simply altitude profiles (usually in steady state) of trace gas mixing ratios. This direct approach was unworkable for intercomparison of 2-D models; there are simply too many differences of formulation to permit a definitive standardized input dataset. Instead we chose to ask each investigator to simulate the photochemistry of the recent atmosphere (circa 1980), the time for which we have the most extensive observations available. Other "standard experiments" focused on particular processes in the model will be undertaken for future intercomparisons.

In order to compare and interpret complex model experiments one needs measures of model sensitivity to the various parameterizations and processes. Among models of common transport formulation (e.g. RMC models) one can directly compare the wind fields and eddy diffusion coefficients fields with some confidence in interpreting their influence on constituent distributions. This is not the case when comparing RMC models to Classical Eulerian (CE) models; then one can only compare net transport fluxes and tracer distributions in assessing the model's transport properties. In comparing such distributions the transport effects are involved with chemistry effects in a way which depends on the local photochemical lifetime of the tracer. This lifetime, in turn, varies with location in the model grid and with season during the simulation. One must therefore be cautious in interpreting such intercomparisons.

Much of the discussion of transport treatments at the Workshop focused on the process of obtaining a residual mean circulation (although results obtained using a Classical Eulerian transport model were also shown and will be discussed below). In the past, and for many of the results presented here, models used temperatures from one source, heating rates from one or more other unrelated sources, and eddy mixing coefficients which were uniform in latitude and time. A conclusion of the Workshop was that this is not a justifiable approach. Within the RMC formulation, temperature, wind fields and eddy mixing are not independent, but should instead be treated in a coupled, self-consistent way, although there are probably several equally viable treatments.   Plumb and Mahlman (1987) have shown that the RMC provides a reasonable approximation to the transport circulation in the stratosphere. Edmon et al. (1980) have shown that the RMC can be solved for in terms of the eddy forcing and diabatic heating. The eddy forcing can be written in terms of a potential vorticity flux, and this flux can be specified in terms of a horizontal diffusion coefficient (K_{yy}). Hence, the RMC, horizontal diffusion, and diabatic heating are mutually dependent. The closure problem arises from the need to specify at least two of these terms in order to derive the third. Usually the diabatic heating is calculated in the model, so either specification or parameterization of eddy diffusion determines the RMC. However, without additional information (from a 3-D model, a treatment of wave propagation through the mean flow, or some other source), it is not possible to compute a full self-consistent response of the transport properties and temperature distribution of the atmosphere to chemical perturbations within the 2-D formulation.

The present level of "coupling" of the advective and diffusive transport of 2-D models is to derive the self-consistent fields for the current atmosphere based on observations. (There are also 2-D models based on zonal averaging of GCM transport fields, but no results from such models were presented at the Workshop). The two approaches discussed at the Workshop were: i) to compute the RMC winds for observed temperature and constituent fields and use potential vorticity (derived from the associated

eddy motions) as a tracer in order to deduce the horizontal eddy coefficients (Newman et al. 1986) and ii) to specify the annual cycle of the zonal mean temperature and compute from this the heating and the associated RMC, and then compute the zonal momentum forcing required to balance the zonal momentum equation (Tung and Yang, 1988). Both approaches depend on temperature observations. It was the general consensus of the workshop participants that available temperature data have neither the accuracy (-1°K) nor the vertical resolution (- 5 km or better) required using either approach.

The most general illustration of this problem was the notable lack of improvement in simulations of trace species distributions in a model based on contemporary temperature data as compared to the distributions in models based on older data. Several models based on distributions of net heating from Murgatroyd and Singleton (1961) [rescaled in various ways to merge with other datasets] were able to simulate long-lived trace species distributions fairly well, while the circulation derived by Rosenfield et. al. (1987) from NMC temperature data, using a modern heating code, was clearly too strong. Moreover, including the "self-consistent" eddy coefficients derived by Newman et. al. (1986) from the same data did not alleviate the problem.

Section 2.4   Conclusions from an Intercomparison of the Species Distributions

Section 2.4.1   Source gases

As noted above the circulation of Rosenfield et. al. (1987) [hereafter the NMC circulation] appears to be too strong, at least during some seasons. Specifically it transports air upward too rapidly in the tropics and downward too rapidly at high latitudes. This results in mixing ratios for N_2O and CH_4 which are larger than those obtained from SAMS by as much as a factor of two at some seasons in the tropical stratosphere above 10 mbar (fig. 2-1). The slopes of the isopleths are also too steep, although this effect can be reduced by using the spatially variable self-consistent eddy coefficients. The frequently observed double-peaked distribution in these species could be simulated in one CE model (Gray and Pyle, 1987) by specifically imposing a semi-annually varying flux, and thus others were unable to reproduce this feature in long term simulations, although Solomon et al. (1986) had some success using circulations based on the specific temperatures as measured by LIMS during SAMS observations.

Section 2.4.2   Odd Nitrogen

RMC models appear to require a source of odd nitrogen in the upper troposphere, perhaps attributable to lightning (Ko et al. 1986; Jackman et al. 1987). The alternative is to use much larger eddy-diffusion coefficients in the lower stratosphere (15-25 km) than those currently believed reasonable, [i.e. $K_{yy} > 10^{10}$ vs. an average value of -3 x 10^9]. This would reduce the latitude contrast in column O_3 and HNO_3 however. The odd nitrogen shortfall did not appear in the CE model of Gray and Pyle, in which the ratio of diffusion to advection in the lower stratosphere is substantially larger.

There is a general problem in all models with the seasonal behavior of HNO_3. In the models the mixing ratio maximum in the summer hemisphere is larger than that in the winter hemisphere, while in the LIMS measurements the opposite is observed (fig. 2-2). It has been suggested (Austin et al. 1986; Jackman et al. 1987) that this implies missing chemistry in the models. The effect of the missing chemistry would be to convert N_2O_5 into HNO_3 during the polar night, perhaps on the surface of aerosols or in cloud droplets.

Section 2.4.3   Active Chlorine

All models show a latitude dependence of the partitioning of chlorine among HCl, ClO, $ClONO_2$ and HOCl. This is especially notable in the 35-45 km range, where active chlorine has its maximum impact as a catalyst for ozone and HCl is at minima. This maxima for Cl_x loss of ozone occurs at

high latitudes in both hemispheres (see fig 2-3). As noted by Solomon et al. (1985) this latitudinal variation depends primarily on the methane distribution. The methane isopleth slopes, in turn, depend on the ratio of advection to diffusion in the model.

The major differences among model Cl_x distributions occurred in polar night, and were caused by different schemes for treating polar night chemistry. These different schemes include computation of production and loss for night conditions, imposed nighttime photochemical equilibrium, and "freezing" the chemistry in polar night (i.e. no computation of changes in species concentrations). These differences probably also affect NO_x in polar night. While the several schemes appear to give similar long-term behavior (e.g. annual cycles at mid-latitudes) they produce substantially different latitudinal gradients at the polar terminator. Such gradients in model distributions must be treated with caution.

Section 2.4.4 Ozone

Peak ozone mixing ratios were similar in all models and consistent with available satellite data (i.e. 9-11 ppm at the maximum). The overall morphology, however, differed according to the transport used. The NMC circulation produced too much downward and poleward slope of the isopleths in the middle and lower stratosphere, as compared to observations.

There is still a general problem with modelled ozone mixing ratios above about 45 km altitude. The model values are consistently too low. This is a longstanding problem with both 1-D and 2-D models, and may derive from shortcomings in photolysis calculations, incorrect chemical kinetic data, incorrect temperatures or something not yet thought of. Jackman noted that, as a consequence, computed photolysis rates can be substantially different (up to 40% in some cases) from those obtained when observed ozone distributions are imposed.

Section 2.5 Perturbation Assessments

Two groups (Oslo and AER) compared ozone depletion assessment calculations, in order to focus on depletion to date (i.e. trend detection in the current atmosphere). While the calculations agree that the earliest and greatest effect would be at high latitudes and at 40-45 km altitude, the estimates presented for maximum local ozone depletion to date differed by a factor of two. The differences do not appear in the computed column depletions. The major differences between the two calculations were the treatment of temperature changes due to increasing CO_2, and the distributions of CH_4 in the models. The latter appeared to be the major effect, influencing both the latitude dependence of ozone depletion in the upper stratosphere, and the projected increase in ozone in the tropical lower stratosphere. The CH_4 distributions, in turn, are sensitive to the transport characteristics of the models. The importance of temperature feedback was more difficult to assess, given the doubts previously expressed about the accuracy of available temperature data in the upper stratosphere. In any case the treatment of temperature feedback was purely photochemical; the importance of dynamical feedback remains unknown.

Section 2.6 Coupled Models

In the context of this Workshop, coupled models are those which attempt to compute temperature, circulation and/or diffusion coefficients, radiative heating and photochemistry, all in an internally self-consistent manner. As noted above, this always requires some additional assumption about temperature or the momentum forcing in order to close the system of equations.

Tung presented preliminary calculations of the sensitivity of the ozone column to perturbations of the lower stratospheric net heating distribution. These suggested as much as a 4% change in column ozone for a 1% change in heating. Because this region is close to radiative equilibrium with large and nearly cancelling heating and cooling terms, the uncertainty in a model heating calculation is likely to be much larger than 1%. This suggests that a detailed comparison of the radiation codes used in models should be undertaken.

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Hitchman showed results for a model in which the meridional diffusitivity and meridional circulation driven by Rossby waves were parameterized by including an equation for Rossby wave activity. The distribution of Rossby wave activity is determined by model zonal winds. The parameterized transport evolves with the zonal winds. This allows for studying feedbacks among temperature, wave driving and tracer distributions.

Section 2.7 Summary

The assessment results are in qualitative agreement with each other (and with previous results) that there is a strong seasonal and latitudinal dependence in the O_3 response. Additional 2-D results will help us in interpretation of data and 1-D model results.

One conclusion of the workshop was that, within the RMC formulation, temperature, wind fields and eddy mixing are not independent, but should instead be treated in a coupled, self-consistent way. Despite the current efforts, a fully self-consistent treatment of the response of the transport properties and temperature distributions of the atmosphere to chemical perturbations within the 2-D formulation is not yet available. It is likely that one would have to depend on additional information from a 3-D model for treatment of wave propagation through mean flow and parameterization of the eddy forcing in order to formulate the approach.

We know that the models used to date have neglected processes (changes in temperature and circulation due to changes in ozone) which may well affect model predictions. Until we have gained more experience with depletion estimates in coupled models, we cannot reach reliable quantitative conclusions as to impact of the neglected feedback processes on the predicted depletion.

Section 2.8 Upper Atmosphere Pilot Database

As a general facility for comparison of model species distributions to each other and to observed distributions (or intercomparison of observations) a remotely accessible database has been established at NASA's Langley Research Center. The participants in the Workshop have "deposited" their model outputs into this database where they are available for continuing intercomparison. Eventually, as additional model studies are published in the literature, the associated model species distributions will be made available in a publicly accessible section of the database. For the moment the publicly accessible portion contains only observational information. Non-Workshop-Participants who are interested in using the portion of the database containing model output are encouraged to contact the participating investigators.

This database is intended to be a community resource, and readers are encouraged to use it and suggest changes and improvements. For information, contact Dr. Robert Seals, Jr., MS401A, NASA/Langley Research Center, Hampton, VA 23665, (804) 864-2696. The data currently available is shown in Table 2-1.

Table 2-1.

Assorted balloon profiles
  N_2O, H_2O, CO, O_3, NO_2, HNO_3, NO, COS, HF, HCl, CH_4

LIMS	November 78 - May 79
H_2O, HNO_3, NO_2, O_3	
SAMS	January 79 - December 79
CH_4, N_2O	
SBUV	October 78 - September 84
O_3	

Workshop Models:

  AER (Jan. 85; Apr. 85)
  CNRM (Mar. 80; Dec. 80)
  Dupont (Jan. 80; Apr. 80)
  GSFC (Apr. 80; Jan. 81)
  NOAA/NCAR (Mar. 84; Dec. 84)
  CAMBRAL (Dec. 79; Apr. 80)

Section 2.9 <u>References</u>

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Solomon, S., R. R. Garcia and F. Stordal, Transport processes and ozone perturbations, <u>J. Atmos. Sci.</u>, <u>90</u>, 12,981-12,989, 1985.

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WMO, Atmospheric Ozone 1985, <u>Rept. No. 16</u>, Global Ozone Research and Monitoring Project, Geneva, 1986.
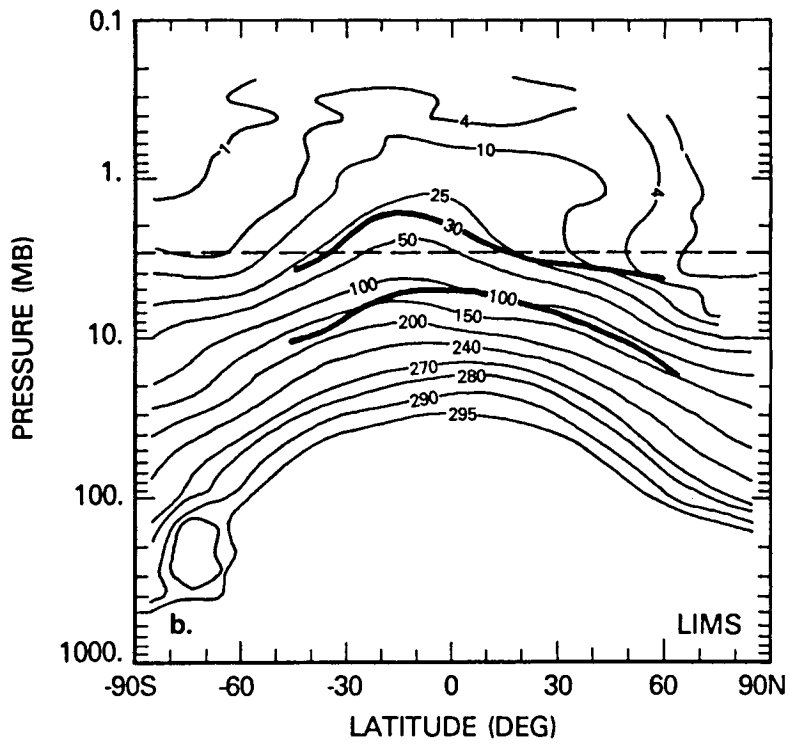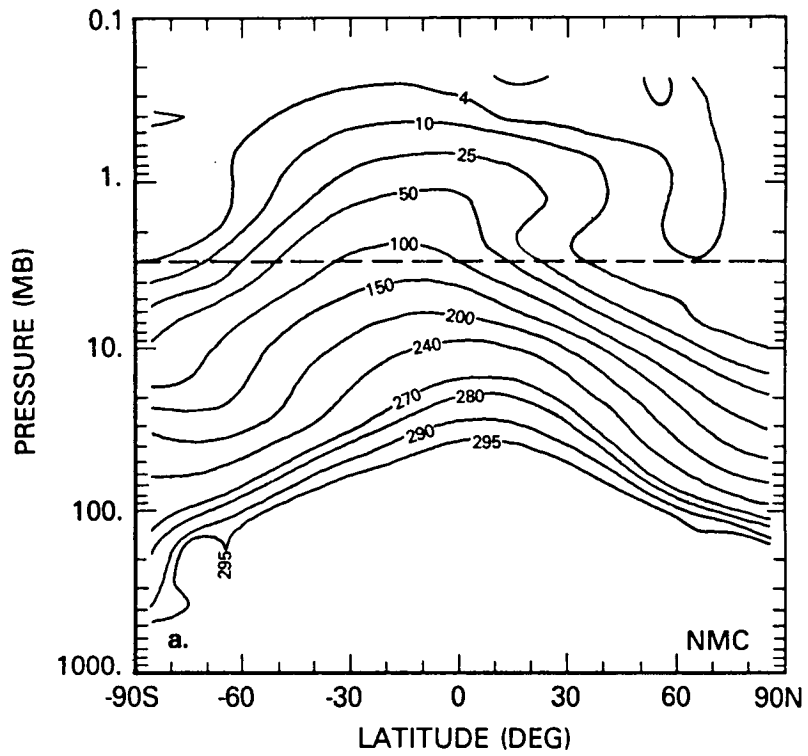
N20 IN PPBV

Figure 2-1. N_2O distributions for January derived from the GSFC model using NMC-derived and LIMS-derived circulations. Heavy contours are SAMS observations. Dashed line highlights the 3 mbar level for comparison.
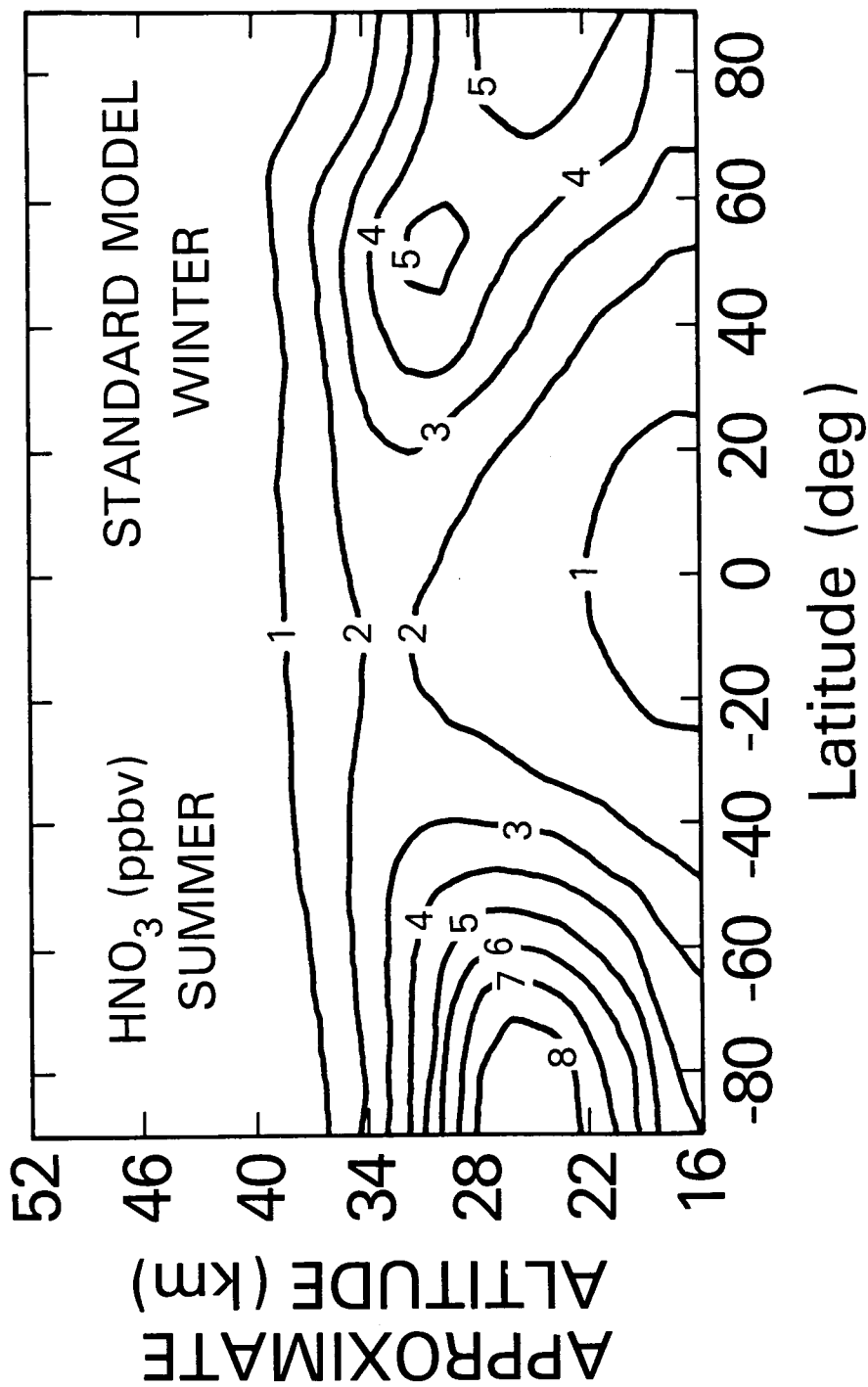
Figure 2-2. a) Calculated HNO₃ distribution at the end of December from the Garcia - Solomon model.
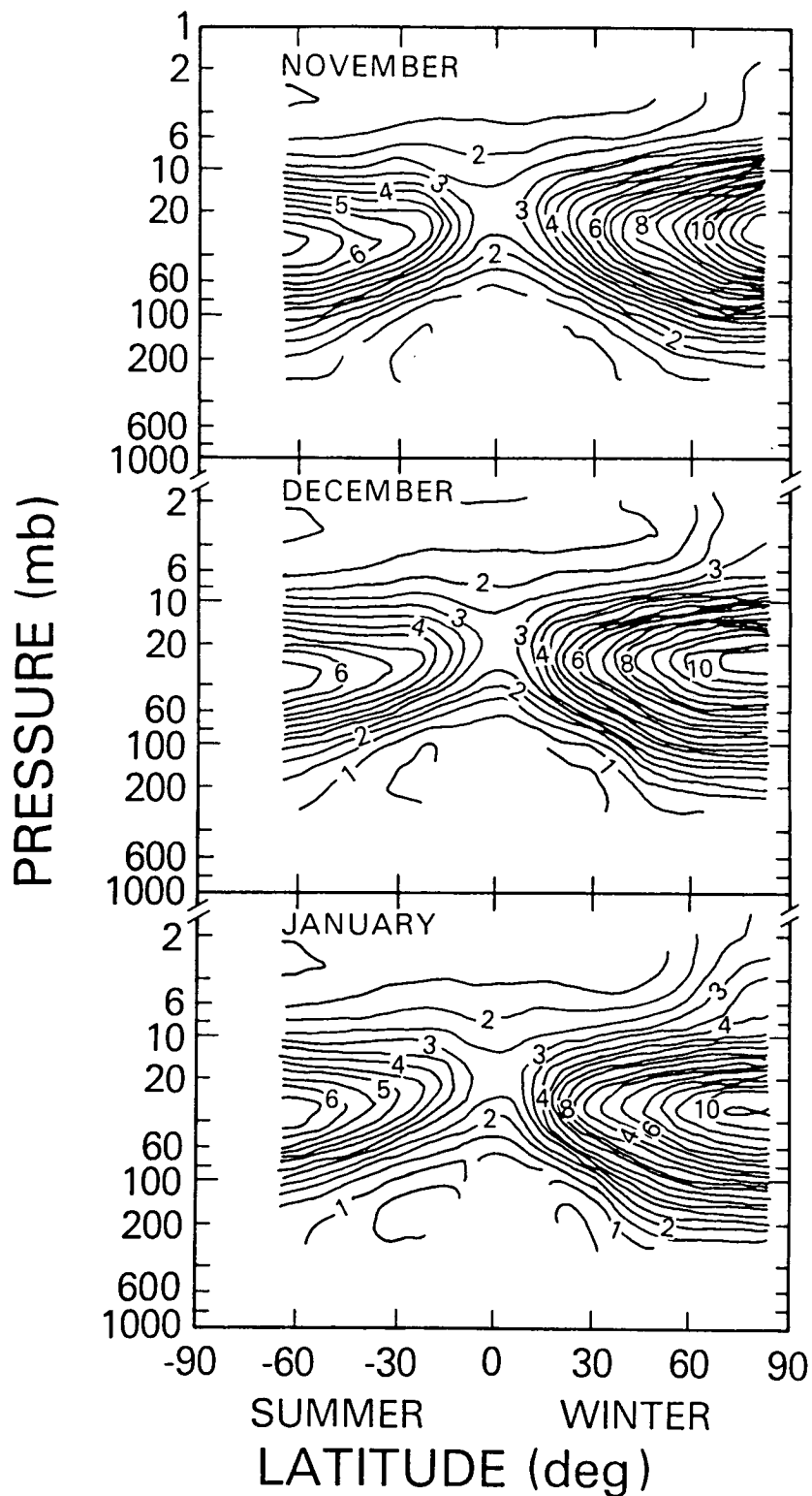
HNO₃ MIXING RATIO (ppbv)

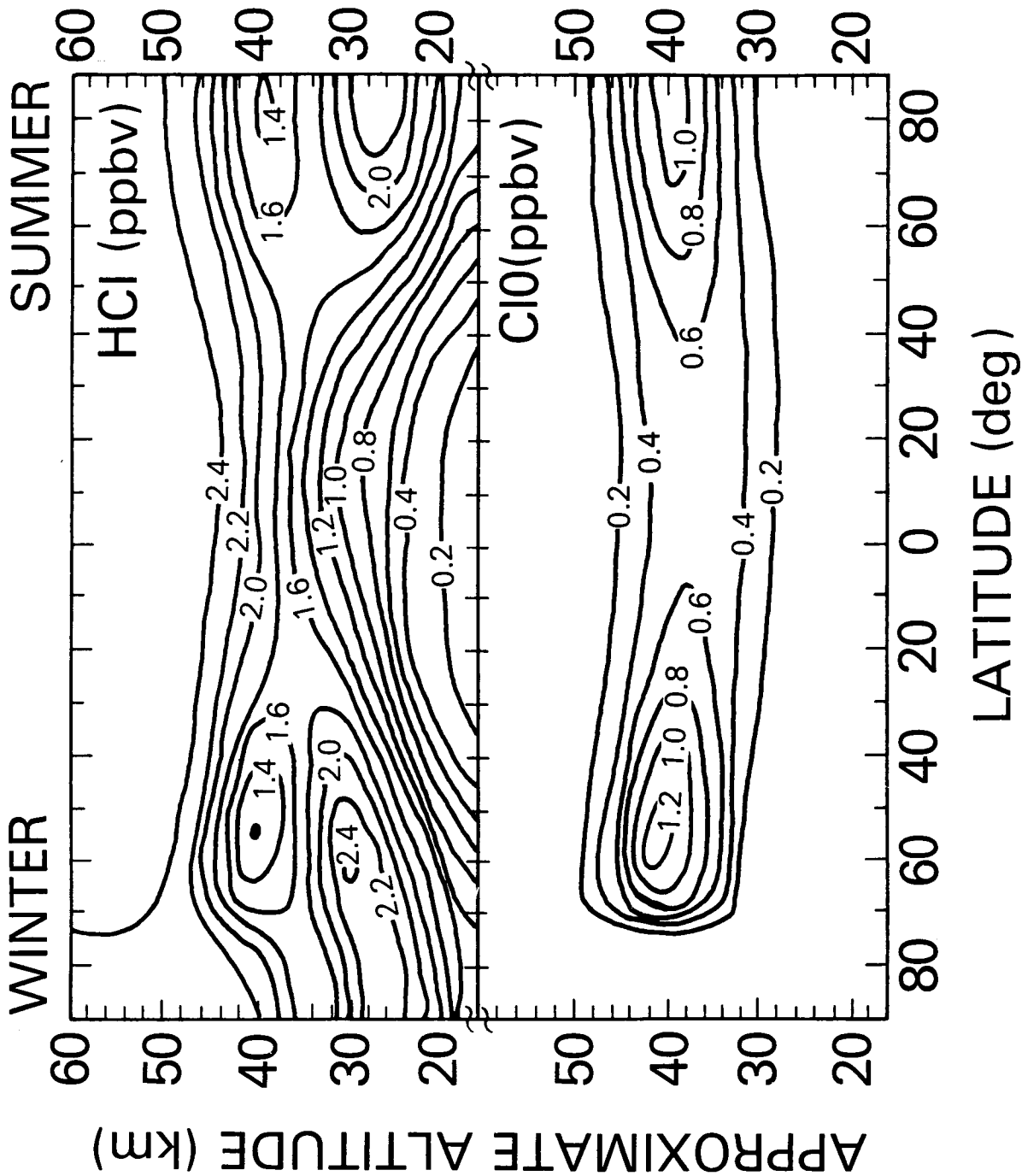Figure 2-2. b) Monthly and zonally averaged HNO₃ distributions observed by LIMS.

Figure 2-3. Contour plots of HCl and ClO near solstice (noon values derived from the Garcia-Solomon model).