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Analysis of Atmospheric Spectra for Trace Gases

Investigators and Institutions

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Abstract of Research Objectives

The objective of this work is the comprehensive analysis of high-resolution atmospheric spectra recorded in the middle-infrared region to obtain simultaneous measurements of coupled parameters (gas concentrations of key trace constituents, total column amounts, pressure, and temperature) in the stratosphere and upper troposphere. Solar absorption spectra recorded at 0.002 and 0.02 cm⁻¹ resolutions with the University of Denver group's balloon-borne, aircraft-borne, and ground-based interferometers and 0.005 to 0.01 cm⁻¹ resolution solar spectra from Kitt Peak are used in the analyses.

Summary of Progress and Results

The major recent focus of this work has been the analysis of the very high $(0.002 \text{ to } 0.003 \text{ cm}^{-1} \text{ FWHM})$ resolution stratospheric solar spectra recorded during The spectra reveal many new features of several three recent balloon flights. important trace gases, such as HNO_3 and COF_2 , as well as new details concerning the absorptions by $CLONO_2$ and HO_2NO_2 . Comparison of the new spectra with lineby-line simulations shows that previous spectral line parameters are often inadequate, and that new analysis of high resolution laboratory and atmospheric spectra and improved theoretical calculations will be required for many bands. Preliminary versions of several sets of improved line parameters have been developed and compared with the balloon-borne spectra. A laboratory analysis of the ν_6 band of COF₂ has been completed. Isotopic ratios of ${}^{16}O^{16}O^{18}O^{18}O^{16}$ and ¹⁶O¹⁸O¹⁶O relative to normal ozone have been measured based on recent improvements in ozone line parameters in the 10- μ m region. Normalized to standard terrestrial isotopic ratios in ozone, both forms of heavy ozone are enriched above 37 km altitude with about a factor of two larger enhancement in ${}^{16}O{}^{18}O{}^{18}O{}$ than ${}^{16}O{}^{18}O{}^{16}O{}^{18}O{}^{16}O{}^{16}O{}^{18}O{}^{16}O{}^{16}O{}^{16}O{}^{18}O{}^{16}O$

In preparation for the Network for the Detection of Stratospheric Change, $0.02-cm^{-1}$ resolution solar spectra recorded at Mauna Loa have been analyzed. Simultaneous total columns have been determined for 13 atmospheric gases, and the daytime diurnal variations of the NO and NO₂ total columns have been measured. The results indicate that Mauna Loa is a favorable site for infrared monitoring of atmospheric gases.

Analysis of the Kitt Peak ground-based solar spectra has continued. A series of 19 spectra recorded during the night using the Moon or during the day using the Sun as a source have been used to measure the daytime and nighttime variation of the NO₂ total column. A continuous increase is observed during the day (lifetime about 10.4 hours) followed by a rather rapid decrease during the night. At sunrise the NO₂ total column drops by about a factor of three. The measurements have been compared with values calculated with a 1-D diurnal photochemical model. Spectra recorded between December 1980 and May 1988 show that the CHClF₂ (CFC-22) total column increased at an average annual exponential rate of 7.8% \pm 1.0% (2 σ). Compared with other atmospheric data, these measurements indicate that CFC-22 is increasing at a more rapid rate than either CFC-11 or CFC-12, the two most abundant chlorofluorocarbons, but that the rate of CFC-22 increase is likely to have declined over the past few years. A systematic discrepancy between the absolute values of infrared and in situ CFC-22 measurements is noted.

Journal Publications (1988-1989)

- Rinsland, C. P., A. Goldman, F. J. Murcray, F. H. Murcray, D. G. Murcray, and J. S. Levine: Infrared Measurements of Increased CF₂Cl₂ (CFC-12) Absorption Above the South Pole, <u>Appl. Opt.</u> <u>27</u>, 627-630, 1988.
- Flaud, J.-M., C. Camy-Peyret, J. W. Brault, C. P. Rinsland, and D. Cariolle: Nighttime and Daytime Variation of Atmospheric NO₂ from Ground-Based Infrared Measurements, <u>Geophys. Res. Lett.</u> 15, 261-264, 1988.
- Goldman, A., F. J. Murcray, F. H. Murcray, D. G. Murcray, and C. P. Rinsland: Measurements of Several Atmospheric Gases Above the South Pole in December 1986 from High Resolution 3- to 4-μm Solar Spectra, <u>J. Geophys. Res.</u> <u>93</u>, 7069-7074, 1988.
- 4. Rinsland, C. P., A. Goldman, F. J. Murcray, F. H. Murcray, and D. G. Murcray: Infrared Measurements of Atmospheric Gases Above Mauna Loa, Hawaii, in February 1987, <u>J. Geophys. Res.</u> <u>93</u>, 12607-12626, 1988.
- 5. Goldman, A., F. J. Murcray, F. H. Murcray, D. G. Murcray, and C. P. Rinsland: Quantification of Several Atmospheric Gases from High Resolution Infrared Solar Spectra Obtained at the South Pole in 1980 and 1986, <u>Mikrochim. Acta</u> (Wien) 2, 409-415 (1988).
- Rinsland, C. P., D. W. Johnson, A. Goldman, and J. S. Levine: Evidence for a Decline in the Atmospheric Accumulation Rate of CHClF₂ (CFC-22), <u>Nature</u> <u>337</u>, 535-537 (1989).
- Murcray, F. J., A. Matthews, A. Goldman, P. Johnston, and C. P. Rinsland: NH₃ Column Abundances over Lauder, New Zealand, <u>J. Geophys. Res.</u> <u>94</u>, 2235-2238, 1989.
- Goldman, A., F. J. Murcray, D. G. Murcray, J. J. Kosters, C. P. Rinsland, J.-M. Flaud, C. Camy-Peyret, and A. Barbe: Isotopic Abundances of Stratospheric Ozone from Balloon-Borne High Resolution Infrared Solar Spectra, J. Geophys. Res. 94, 8467-8473, 1989.
- 9. Goldman, A., F. J. Murcray, R. D. Blatherwick, J. J. Kosters, F. H. Murcray, D. G. Murcray, and C. P. Rinsland: New Spectral Features of Stratospheric Trace Gases Identified from High Resolution Infrared Balloon-Borne and Laboratory Spectra, J. Geophys. Res., in press.
- 10. Goldman, A., C. P. Rinsland, R. D. Blatherwick, and F. S. Bonomo: Spectroscopic Line Parameters for the ν_6 Band of Carbonyl Fluoride (COF₂), submitted to <u>Appl. Opt.</u>
- 11. Flaud, J.-M., C. Camy-Peyret, C. P. Rinsland, V. Malaty Devi, M. A. H. Smith, and A. Goldman: Improved Line Parameters for Ozone Bands in the 10 μ m Spectral Region, submitted to <u>Appl. Opt.</u>

III. THEORETICAL STUDIES

- A. GLOBAL MODELLING OF STRATOSPHERIC CHEMISTRY
- B. MODELLING PHOTOCHEMICAL PROCESSES
- C. STRATOSPHERIC DYNAMICS

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A. GLOBAL MODELLING OF STRATOSPHERIC CHEMISTRY

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- A. Zonally-averaged Model of Dynamics, Chemistry and Radiation for the Atmosphere
- B. Principle Investigators : Nien-Dak Sze and Malcolm Ko
 - Co-investigators : Arthur Y. Hou, Jose M. Rodriguez, Hans-R. Schneider and Debra K. Weisenstein
 - Atmospheric and Environmental Research Inc., 840, Memorial Drive, Cambridge, MA 02139

C. Abstract of Research Objective

The overall goal of the project is to obtain an understanding of the processes that control the distribution and abundance of stratospheric ozone and its sensitivity to either natural or anthropogenic influences. The scientific objectives, which are designed around the two-dimensional zonal mean (2-D) modeling capability at AER, are :

- To assess the limitation of 2-D models, to refine and enhance our current (2-D) modeling capabilities and understanding of the stratosphere through model simulations and validation of model results using observed data.
- To develop an interactive 2-D model with interactive chemistry, dynamics and radiation.
- To assess the susceptibility of stratospheric ozone to natural and anthropogenic perturbations.
- To study the processes that give rise to the Antarctic Ozone Hole and assess their global impact.

D. Summary of Progress and Results

Ozone Budget

We used result from the 2-D model to clarify the roles of chemistry and transport in determining the concentration of O_3 in the 2-D model (Ko et al, 1989). We found that at the tropical lower stratosphere, the concentration of O_3 is determined by a balance between chemical production and transport out of the region. At high latitudes, the balance is between local chemical removal and transport into the region. Our study help to explain the response of model ozone to chemical perturbation and clarify the limitation of 1-D model results.

Assessment Calculations and Ozone Depletion Potentials

The calculated O_3 behavior in the future atmosphere from our assessment calculations were used in a study to examine the effect of redistribution of O_3 on climate (Wang et al, 1989). We performed a number of assessment calculations and provided inputs for the preparation of several reports including the NASA Reference Publication report 1208, "Present State of Knowledge of the Upper Atmosphere 1988 : An Assessment Report" and the UNEP/WMO report. We also used the 2-D model to calculate the Ozone Depletion Potential of a number of CFC substitutes and examined how the calculated values are affected by the transport parameters in the model.

Interactive Model and Dynamics

The interactive model is now operational. We have used the version with simplified chemistry to study the model sensitivity to Kyy (Schneider et al 1989) and the feedback effects from change in O_3 . Our model simulations showed that the temperature and dynamics feedback from change in local heating

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could compensate for about 1/6 of the calculated O₃ decrease. The version of the model with full chemistry has been used to simulate the present day atmosphere and perform a number of steady state assessment calculations. The emphasis of the work is related to our theoretic study that clarify their role of Kyy in controlling the diabatic circulation (Hou and Ko, 1989).

Antarctic Ozone

Part of 1988 was spent in the analysis of the data from the Airborne Antarctic Ozone Experiment. Analysis of the data resulted in three publications that discussed the effect on global O₃ content from export of O₃-poor air from the vortex, the so-called dilution effect (Sze et al, 1989), the comparison of simulated trace gas distributions in the vortex with the AAOE observations (Rodriguez et al, 1989) and the decadal trend of the ozone behavior in the polar vortex (Ko et al, 1989).

E. Journal Publications

- Rodriguez, J.M., M. K. W. Ko, and N. D. Sze (1988) Antarctic chlorine chemistry: possible global implications. <u>Geophys. Res. Lett.</u>, <u>15</u>, 257-260.
- Hou, A.Y., and M. K. W. Ko (1989) Ageostrophic effects on the stratospheric residual circulation and tracer distributions. <u>J. Atmos. Sci.</u>, <u>46</u>, 1396-1406.
- Schneider, H. R., M. K. W. Ko, N. D. Sze, G.-Y. Shi, and W.-C. Wang (1989) An evaluation of the role of eddy diffusion in stratospheric interactive 2-D models. <u>J. Atmos. Sci.</u>, <u>46</u>, 2079-2093.
- Ko, M. K. W., N. D. Sze, and D. Weisenstein (1989) The roles of chemical and dynamical processes in determining the stratospheric concentration of ozone in one-dimensional and two-dimensional models. <u>J. Geophys. Res.</u>, <u>94</u>, 9889-9896.
- Wang, W.-C., G. Molnar, M. K. W. Ko, S. Goldenberg, and N. D. Sze (1989) Atmospheric trace gases and global climate: a seasonal model study. <u>Tellus</u>, in press.
- Ko, M. K. W., J. M. Rodriguez, N. D. Sze, M. H. Profitt, W. L. Starr, A. Krueger, E. V. Browell, and M. P. McCormick (1989) Implications of AAOE observations for proposed chemical explanations of the seasonal and interannual behavior of Antarctic ozone. To appear in <u>J. Geophys. Res</u>.
- Rodriguez J. M., M. K. W. Ko, N. D. Sze, S. D. Pierce, J. G. Anderson, D. W. Fahey, K. Kelly, C. B. Farmer, G. C. Toon, M. T. Coffey, L. E. Heidt, W. G. Mankin, K. R. Chan, W. L. Starr, J. F. Vedder, and M. P. McCormick (1989) Nitrogen and halogen species in the spring Antarctic stratosphere: comparison of models and AAOE observations. To appear in <u>J. Geophys. Res</u>.
- Sze, N. D., M. K. W. Ko, D. K. Weisenstein, and J. M. Rodriguez (1989) Antarctic ozone hole: possible implications for ozone trends in the Southern hemisphere. To appear in <u>J. Geophys. Res</u>.

- A. Acquisition and Utilization of Archived Satellite Data from the NASA Upper Atmospheric Research Program : Validation and Enhancement of a Two-dimensional Zonal-mean Model
- B. Principle Investigators : Malcolm K. Ko and Nien-Dak Sze Co-investigator : Arthur Y. Hou, Hans-R. Schneider and Debra K. Weisenstein Atmospheric and Environmental Research Inc., 840, Memorial Drive, Cambridge, MA 02139

C. Abstract of Research Objective

The objective of the program is to acquire satellite data from the NASA Upper Atmosphere Research Program and to organise them in a form that is suitable for use in support of the two-dimensional modeling work at AER.

D. Summary of Progress and Results

Acquisition of Data

We have acquired and organised five data sets. These are the BUV O_3 data; the SBUV O_3 data; the TOMS O_3 data; the LIMS data on temperature, O_3 , NO_2 , H_2O , HNO_3 and geopotential height; and the SAMS data on N_2O and CH_4 . The data were interpolated into the AER model grid and processed that they are suitable for use as input for model studies and for comparison with model results.

Calculation of Diabatic Circulation Using Observed Temperature and $\ensuremath{\texttt{O}}_3$

The zonal-mean O_3 mixing ratio from SBUV was used together with the observed temperature from NMC to obtain the heating rate using the AER radiation code. A seasonal zonal-mean circulation was calculated from the diabatic heating rates.

Interannual Variation of Ozone

Using the O_3 concentrations and observed monthly mean temperature from NMC for the four year period (1978-1982), radiative heating rates were computed for each month of the four years. The circulations diagnosed from the heating rates were used in the 2-D chemistry-transport model to calculate the O_3 behavior. The model calculated inter-annual fluctuations was compared with the observation. Our model calculation suggested that the observed interannual variability in O_3 is a response to fluctuations in the transport circulation in the lower stratosphere. Furthermore, the year-to-year variations in the circulation are a results of the temperature fluctuations. Finally, the change in temperature cannot be explained by the fluctuations in O_3 and is more likely a results from the changes in eddy heat transport.

Utilization of N₂O data from SAMS

The atmospheric lifetime of N_2O is determined by the photochemical removal of the gas in the lower stratosphere. Previous calculations using balloon observations of N_2O as data and/or for validation obtained a lifetime for N_2O of about 150-175 years. Data for N_2O is available from the SAMS instrument on Nimbus-7 covering the region from 50°S to 70°N, 25 km to 50 km where 80% of the removal occurs. Using the observed N_2O data to check against the model calculated distribution, we concluded that calculated lifetimes as short as 114 years are consistent with the data.

Photochemical Studies using LIMS data

We incorporated the observed O_3 , H_2O , and temperature from LIMS as input into our diurnal model. In this mode of operation, the values for local temperature, O_3 and H_2O are assigned the observed values and the concentrations for the other long-lived trace gases are taken from previous model simulations. The model is then used to calculate the concentrations of the short-lived species assuming local photochemical equilibrium. The model results are compared with the LIMS observed NO₂ and HNO₃.

Publication in Preparation

Schneider, H-R, M.K.W. Ko, C.A. Peterson and E. Nash, Interannual Variation of Ozone : Interpretation of 4 years of Nimbus 7 SBUV Observations.

Ko, Malcolm, N-D Sze and D. K. Weisenstein, Validation of Atmospheric Lifetimes for Source Gases Using N₂O Data from SAMS.

<u>Studies of the antarctic ozone hole:</u> Analysis of perturbations to global ozone trends

Jose M. Rodriguez, Malcolm K. W. Ko, Nien Dak Sze

Atmospheric and Environmental Research, Inc. 840 Memorial Drive Cambridge, MA 02139

Research Objectives

The general objective of this program is to refine our understanding of the chemistry of the antarctic ozone hole, and to study the impact of polar phenomena (heterogeneous chemistry, dilution effect, denitrification) on the global ozone trends. The specific goals are:

- Further studies of the dilution of the antarctic ozone loss using our two-dimensional chemistry transport model; comparison to other model results and observational data.
- Incorporation of heterogeneous processes into our 2-D model, both in the polar regions and in the global atmosphere, in a manner consistent with available laboratory data and field measurements.
- Assessment of the impact of heterogeneous reactions both for the present and future atmosphere; assessment of the future behavior of the antarctic ozone hole and its impact on global ozone trends; assessment of the coupling among ozone and temperature perturbations, circulation changes, and dynamical redistribution.

Progress and Results

Our work during the first year has concentrated on three general areas: a) studies of the photochemistry of the Antarctic stratosphere; b) assessment of the impact of high-latitude chemistry on the HO_x and O_3 budgets; c) impact of high-latitude and global heterogeneous chemistry on ozone trends. The main results of our research are as follows:

- We have assessed the impact of new kinetic data for formation and photolysis of $C\ell_2O_2$ on the partitioning of chlorine species and calculated ozone reductions within the Antarctic polar vortex. Calculations indicate that the observed $C\ell O$ and $C\ell NO_3$ column densities near the edge of the vortex are consistent if we adopt the new kinetic data. Decreases in the observed column densities of $HC\ell$ and $C\ell NO_3$ towards the core of the vortex suggest an increase in $C\ell O$ with latitude, with a correspondingly larger calculated reductions of ozone. The ozone reductions calculated with the new kinetic data are still consistent with observations, if we consider the spread in both the ozone and $C\ell O$ measurements and mixing of air within the vortex.
- We have incorporated heterogeneous chemistry in our 2-D model, both on Polar Stratospheric Clouds (PSCs) and on the global sulfate layer.
- Model results indicate that the heterogeneous reaction of $CLNO_3$ with H_2O (ice, aerosol) could be the primary source of HO_x at high latitudes winter (greater than 60°) if the atmosphere has been

depleted in NO_x but not in HNO₃, and if the equivalent first-order rate of this reaction if about 10^{-6} s⁻¹. Inclusion of this reaction in our model increased the calculated HO_x abundances by almost a factor of 10, with corresponding changes in the partitioning between HC*l* and other chlorine species. Ozone loss below 22 km occurred in this case primarily through chlorine and HO_x catalytic cycles.

We have started the assessment of the impact of heterogeneous chemistry by considering two cases: 1) heterogeneous reactions occurring in a denitrified atmosphere on PSCs at high latitudes during winter; 2) heterogeneous reaction of HCl with ClNO₃ occurring year-round in the global sulfate later, with a reaction efficiency of about 10⁻³. Both cases yield calculated ozone trends for the past 20 years consistent with those derived by the NASA Ozone Trends Panel. However, the calculated future ozone trends are dramatically different. Possibility (1) yields ozone reductions in the year 2060 of order 10% relative to 1985 at high latitudes, winter. The assumptions in (2) result in calculated ozone reductions of order 20 - 30% for the same year, season, and latitude. Uncertainties in the kinetic data for heterogeneous reactions indicates the need for further sensitivity studies, and for validation of model results by comparing to data on other trace species (ie., Cl0).

Conference Presentations

- Rodriguez, J. M., M. K. W. Ko, and N. D. Sze (1989) "Impact of new kinetic data for the chemistry of the Antarctic stratosphere," presented at the Spring Meeting of the American Geophysical Union, Baltimore, MD, May 7-12, 1989. EOS, 70, 299.
- Rodriguez, J. M., M. K. W. Ko, N. D. Sze, and D. Weisenstein (1989): "Global implications of heterogeneous chemistry: Assessment utilizing a twodimensional model," presented at the Fifth Scientific Assembly of the International Association of Meteorology and Atmospheric Physics (IAMAP), Reading, England, July 31-August 11, 1989.

Publications

D. W. Fahey, D. M. Murphy, K. K. Kelly, M. K. W. Ko, M. H. Proffitt, C. S. Eubank, G. V. Ferry, M. Loewenstein and K. R. Chan (1989) "Measurements of nitric oxide and total reactive nitrogen in the Antarctic stratosphere: Observations and chemical implications," <u>J. Geophys. Res.</u>, in press.

Publications in preparation

- Rodriguez, J. M., M. K. W. Ko and N. D. Sze (1989): "Partitioning of chlorine species inside the Antarctic polar vortex."
- Rodriguez, J. M., M. K. W. Ko, N. D. Sze and D. Weisenstein (1989): "Global implications of heterogeneous chemistry."

Research Summary 1988-1989

A. Title of Research Task

Interactions of Atmospheric Chemical, Radiative, and Dynamical Processes: Research Studies with and Further Development of the LLNL Two-Dimensional Global Atmospheric Model

B. Investigators and Institutions

Principal Investigator: Dr. Donald J. Wuebbles

Co-Investigators:	Dr. Peter S. Connell
	Dr. Keith E. Grant
	Dr. Douglas E. Kinnison

C. Research Objectives

The primary goals of this project are the further development of the LLNL twodimensional chemical-radiative-transport model of the troposphere and stratosphere, and the application of this model to research studies on the middle atmosphere. Model capabilities are being extended towards improving understanding of the key processes that control the distribution of ozone and other important species in the global atmosphere. Research studies are primarily oriented at assessing the past and possible future changes in ozone from natural and human-induced causes, and to improve understanding of observations of global trace constituent distributions.

D. Progress and Results

The two-dimensional model has been applied to a number of research studies during 1988 and 1989. LLNL scientists have also participated in several international assessment efforts in support of NASA during this time period. Past trends in ozone and temperature were analyzed with the model for the Trends Panel Report (we also contributed to the writing of this report being published through NASA and other organizations). For the recent Scientific Assessment of Stratospheric Ozone: 1989 (being published by WMO), we not only provided model calculations for trace gas scenario effects on ozone and an analysis of ozone depletion potentials for CFCs and other compounds, but also coordinated the preparation and writing of one of the four chapters. In 1988, we helped coordinate and participated in an international two-dimensional intercomparison of atmospheric models sponsored by NASA.

Research studies with the two-dimensional model include: an analysis of trends in ozone and temperature over the past thirty years, including a careful evaluation of the possible effects on ozone resulting from atmospheric nuclear testing in the early 1960s; an analysis and sensitivity study of potential effects of high speed commercial aircraft on stratospheric ozone; an analysis of carbon-14 and other tracers produced from nuclear tests to determine their usefulness for validating the treatment of troposphere-stratosphere exchange processes in the 2-d model; and an analysis of the 11-year solar cycle for its effects on upper stratospheric ozone and temperature.

The two-dimensional model has been continued to be improved and refined. Additional layers have been added to the model to extend it into the lower mesosphere and to improve the resolution in the troposphere. The solar and infrared radiative submodels have extensively revised to provide improved treatment of scattering and cloud-related processes. Determination of upper stratospheric cooling rates has also been improved. At the same time, computational speed has been improved, such that the current model runs as fast as earlier versions.

E. Publications

- Connell, P. S., and D. J. Wuebbles, "Evaluating CFC Alternatives from the Atmospheric Viewpoint," Air and Waste Management Assoc. paper 89-5.7, 1989.
- DeLuisi, J. J., D. U. Longenecker, C. L. Mateer, and D. J. Wuebbles, "An Analysis of Northern Middle-Latitude Umkehr Measurements Corrected for Stratospheric Aerosols for 1979-1986", J. Geophys. Res. 94, 9837-9846, 1989.
- Grant, K. E., R. G. Ellingson, and D. J. Wuebbles, "Sensitivity of a Two-Dimensional Chemistry-Transport Model to Changes in Parameterizations of Radiative Processes", in *IRS '88: Current Problems in Atmospheric Radiation*, J. Lenoble and J-F. Geleyn, editors, A. Deepak Publishing, Hampton, Va., 1989.
- Johnston, H., D. E. Kinnison, and D. J. Wuebbles, "Nitrogen Oxides from High Altitude Aircraft: An Update of Potential Effects on Ozone", J. Geophys. Res. 94, in press, 1989.
- Kinnison, D. E., H. Johnston and D. Wuebbles, "Ozone Calculations with Large Nitrous Oxide and Chlorine Changes", J. Geophys. Res. 93, 14165-14175, 1988.
- Reinsel, G. C., G. C. Tiao, S. K. Ahn, M. Pugh, S. Basu, J. J. DeLuisi, C. L. Mateer, A. J. Miller, P. S. Connell, and D. J. Wuebbles, "An Analysis of the 7-Year Record of SBUV Satellite Ozone Data: Global Profile Features and Trends in Total Ozone", J. Geophys Res. 93, 1689-1703, 1988.

Wuebbles, D. J., and D. E. Kinnison, "A Two-Dimensional Model Study of Past Trends in Global Ozone", Proceedings, 1988 Quadrennial Ozone Symposium, in press, 1989.

Wuebbles, D. J., K. E. Grant, P. S. Connell, and J. E. Penner, "The Role of Atmospheric Chemistry in Climate Change", J. Air Pollution Control Assoc. 39, 22-28, 1989.

- A. Two-Dimensional Model Studies of the Middle Atmosphere
- B. R. R. Garcia, National Center for Atmospheric Research, Boulder, CO
 S. Solomon, NOAA / Aeronomy Laboratory, Boulder, CO
 J. T. Kiehl, National Center for Atmospheric Research, Boulder, CO
- C. The two-dimensional model of Garcia and Solomon will be used to study several aspects of radiative-chemical-dynamical coupling in the middle atmosphere. The proposal consists of three components: Improvements and extensions of our present 2D model; studies of radiative/photochemical coupling in the contemporary middle atmosphere; and studies of possible interactions among radiation, dynamics and photochemistry that may be important in the future atmosphere due to changes in CFCs, carbon dioxide, methane, and nitrous oxide.
- **D.** The 2D model has been improved by the addition of an IR transfer model developed by J. Kiehl. This model uses a band formulation to explicitly compute IR heating/cooling rates. The model domain had been extended to include the troposphere. Model dynamics have been reformulated to include explicit solution of the zonal mean momentum equation. The new dynamical formulation should allow studies of tropical dynamics not possible with the previous version wherein the zonal wind was assumed to be in thermal wind balance with the temperature field. A single-wavenumber planetary wave model has been coupled to the 2D model to study seasonal and interhemispheric differences in transport due to planetary wave activity.
- E. Papers on the response of the stratosphere to multiple anthropogenic perturbations $(CFCs + CO_2 + CH_4)$ and on the new model dynamics are in preparation.

NASA RESEARCH SUMMARY

Grant No. NAGW-1605

A. Title of Research Task:

Zonally-Averaged Model of Dynamics, Chemistry and Radiation for the Atmosphere

B. Principle Investigator:

Ka-Kit Tung, Professor of Applied Mathematics, University of Washington

C. Abstract of Research Objectives:

To construct a physically based 2-D model with coupled dynamics, chemistry and radiation; to use such a model to simulate the present date distribution of trace gases in the stratosphere and to assess future change.

D. Summary of Progress and Results:

We have completed the implementation of the diagnostic model using NMC temperature as input from which both the advective and diffusive transports are deduced. We have recently added a narrow-band radiative transfer model, which has an accuracy of better than 10% when compared to the line-by-line calculations. We have also completed the implementation of the chemistry module, with O_x , HO_x , NO_x and CIO_x cycles. The simulation of present date distribution of many species, including ozone, using the coupled model showed great improvements over previous generations of models.

- E. Publications:
 - K.K. Tung and H. Yang: Dynamical component of seasonal and year-to-year changes in Antarctic and global ozone. J. of Geophys. Research, <u>93</u>, 12537-12559, 1988.
 - K.K. Tung and H. Yang: Dynamic variability of column ozone, J. of Geophys. Research, 93, 11123-11128, 1988.
 - H. Yang, K.K. Tung and E.P. Olaguar: Two-D model simulation of ozone climatology and year-to-year variations, in Proceedings of Quadrennial Ozone Symposium, 1988.
 - H. Yang, K.K. Tung and E.P. Olaguar: Nongeostrophic theory of zonally averaged circulation. Part II: E-P fluxes and isentropic mixing coefficients, J. Atmos. Sci., accepted 1989.