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**HIGH RESOLUTION INFRARED DATASETS
USEFUL FOR VALIDATING STRATOSPHERIC MODELS**

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INTRODUCTION

An important objective of the High Speed Research Program (HSRP) is to support research in the atmospheric sciences that will improve our basic understanding of the circulation and chemistry of the stratosphere and lead to an interim assessment of the impact of a projected fleet of HSCTs (High Speed Civil Transports) on the stratosphere. As part of this work, critical comparisons between models and existing high-quality measurements are planned. These comparisons will be used to test the reliability of current atmospheric chemistry models. In this paper, two suitable sets of high-resolution infrared measurements are discussed.

ATMOS/SPACELAB 3 DATASET

The ATMOS (Atmospheric Trace Molecule Spectroscopy) experiment was designed to obtain 0.015-cm^{-1} resolution infrared solar occultation spectra of the atmosphere from which the vertical distributions of a large number of minor and trace molecular constituents of the upper atmosphere could be retrieved. The experiment was flown for the first time in the spring of 1985 as part of the Shuttle Spacelab-3 mission. Nineteen complete atmospheric occultations were recorded, twelve sunsets between latitudes of 25°N and 32°N , and seven sunrises between 45°S and 48°S latitude, on April 29 to May 1, 1985. For an overview of the ATMOS experiment and the results of the Spacelab 3 mission see the paper by Farmer (ref. 1).

The profiles for several dozen atmospheric constituents and pressure and temperature have been retrieved from the ATMOS middle atmosphere data. Because the spectra were recorded with broadband filters, chemically linked molecular species were often measured simultaneously, thus providing a unique opportunity to study the partitioning within key chemical families. The ATMOS/Spacelab 3 results are reviewed below. References which give the retrieved profiles and their uncertainties are cited.

Chlorine and Fluorine Budgets. Stratospheric profiles of 11 chlorine- and fluorine-containing source, sink, and reservoir molecules were derived from the Spacelab 3 measurements. The molecules are CCl_2F_2 (chlorofluorocarbon 12), CCl_3F (chlorofluorocarbon 11), CHClF_2 (chlorofluorocarbon 22), CCl_4 , ClONO_2 , HCl , HF , CF_4 (chlorofluorocarbon 14), COF_2 , CH_3Cl , and SF_6 . Results for the source gases have been reported by Zander et al. (ref. 2). Measurements of the sink gases were reported by Raper et al. (ref. 3). Recently, the profiles of HCl , HF , and ClONO_2 have been revised based on improvements in the spectroscopic database and the processing of the ATMOS spectra (ref. 4). The identification and results for SF_6 are reported in ref. 5.

Odd Nitrogen Budget. Profiles of the following odd nitrogen molecular species were derived from the Spacelab 3 measurements: NO , NO_2 , HNO_3 , HO_2NO_2 , N_2O_5 , and ClONO_2 . The analysis included normalized factors that correct for the rapid diurnal variations of NO and NO_2 at sunrise and sunset. These factors were computed with a photochemical

model. The profiles of N_2O_5 were measured for the first time at both sunrise ($48^\circ S$) and sunset ($28^\circ N$). The profiles are reported in ref. 6, except for the updated measurements of N_2O_5 which are in ref. 7.

Key Minor Gases. The ATMOS profiles of CH_4 , N_2O , CO , H_2O , and O_3 cover a wide region of the middle atmosphere (ref. 8). For example, the H_2O profiles extend from 14 to 86 km and the O_3 profiles cover 14 to 94 km. The ATMOS sunset profiles of CH_4 and N_2O show a fold in their vertical distributions which is probably the result of dynamics. The sunrise profiles do not show the fold. Recently, stratospheric profiles of the isotopic species $H_2^{18}O$, $H_2^{17}O$, HDO , and CH_3D have also been retrieved (ref. 9).

Other Gases. Profiles of the nonmethane hydrocarbons C_2H_6 and C_2H_2 (ref. 10) and the molecules HCN and OCS (ref. 11) have also been reported from the ATMOS/Spacelab 3 observations.

GROUND-BASED MEASUREMENTS OF TOTAL COLUMNS

High-resolution ($\sim 0.01 \text{ cm}^{-1}$) solar absorption spectra recorded with the McMath Fourier transform spectrometer on Kitt Peak (altitude 2.09 km, $31.9^\circ N$, $111.6^\circ W$) have been analyzed to deduce total column amounts of HF on 93 different days and HCl on 35 different days between May 1977 and June 1990 (ref. 12). The results indicate a rapid increase in total HF and a more gradual increase in total HCl with both trends superimposed on a seasonal cycle with an early spring maximum and an early fall minimum. The peak-to-peak amplitudes of the seasonal cycle are equal to 25% for HF and 13% for HCl.

These results are of interest since current estimates indicate that the supersonic fleet may be operating in the early 21st century when the atmospheric concentrations of several key gases will be different than they are today. Sensitivity studies to assess the effects of these aircraft will necessarily require generating scenarios for future emissions including the projected emissions of supersonic and subsonic aircraft. The Kitt Peak measurements provide an opportunity to compare model calculations with a time series of accurate measurements for which there are fairly reliable data on emission histories and photo-oxidation rates for the source molecules. The model-predicted and measured total columns, increase rates, and seasonal cycles can be compared.

Of the two species, HF is better suited for the model-measurement comparisons because there probably are no significant tropospheric HF sources. In contrast, in the boundary layer, HCl is produced primarily by the interaction of SO_4 and NO_3 ions with NaCl in ocean spray, and to a lesser extent by surface anthropogenic emissions, such as the burning of plastics and emissions from certain industrial processes. Because of these sources, it is necessary to specify a nonzero surface level HCl flux in model calculations to simulate total column observations. Previous model-model comparisons showed large scatter in the calculated HCl total columns because of differences in the adopted surface level HCl concentration (ref. 13). Therefore, to

make meaningful comparisons with the Kitt Peak data, the tropospheric contribution will need to be prescribed in the model runs based on the observations, which indicate that the tropospheric contribution is about 15% of the total column.

Additional long-term IR spectroscopic observations of HF and HCl have been obtained from the Jungfraujoch station in the Switzerland (altitude 3.58 km, 46.5°N, 8.0°E). At the present time, R. Zander of the University of Liège and collaborators are reanalyzing the early data and extending the baseline of total column measurements based on recently collected solar spectra. It is unclear whether or not this updated database will be available in time for the upcoming HSRP model-measurement comparisons.

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