

HIGH RESOLUTION INFRARED DATASETS  
USEFUL FOR VALIDATING STRATOSPHERIC MODELS

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514-46  
12029

First Annual High-Speed Research Workshop  
Williamsburg, Virginia  
May 14-16, 1991

## 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  $0.015\text{-cm}^{-1}$  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  $25^{\circ}\text{N}$  and  $32^{\circ}\text{N}$ , and seven sunrises between  $45^{\circ}\text{S}$  and  $48^{\circ}\text{S}$  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  $\text{CCl}_2\text{F}_2$  (chlorofluorocarbon 12),  $\text{CCl}_3\text{F}$  (chlorofluorocarbon 11),  $\text{CHClF}_2$  (chlorofluorocarbon 22),  $\text{CCl}_4$ ,  $\text{ClONO}_2$ ,  $\text{HCl}$ ,  $\text{HF}$ ,  $\text{CF}_4$  (chlorofluorocarbon 14),  $\text{COF}_2$ ,  $\text{CH}_3\text{Cl}$ , and  $\text{SF}_6$ . 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  $\text{HCl}$ ,  $\text{HF}$ , and  $\text{ClONO}_2$  have been revised based on improvements in the spectroscopic database and the processing of the ATMOS spectra (ref. 4). The identification and results for  $\text{SF}_6$  are reported in ref. 5.

Odd Nitrogen Budget. Profiles of the following odd nitrogen molecular species were derived from the Spacelab 3 measurements:  $\text{NO}$ ,  $\text{NO}_2$ ,  $\text{HNO}_3$ ,  $\text{HO}_2\text{NO}_2$ ,  $\text{N}_2\text{O}_5$ , and  $\text{ClONO}_2$ . The analysis included normalized factors that correct for the rapid diurnal variations of  $\text{NO}$  and  $\text{NO}_2$  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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# REPORT DOCUMENTATION PAGE

Form Approved  
OMB No. 0704-0188

Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.

1. AGENCY USE ONLY (Leave blank)		2. REPORT DATE April 1992	3. REPORT TYPE AND DATES COVERED Conference Publication	
4. TITLE AND SUBTITLE First Annual High-Speed Research Workshop			5. FUNDING NUMBERS WU 537-01-22-01	
6. AUTHOR(S) Allen H. Whitehead, Jr., Compiler			8. PERFORMING ORGANIZATION REPORT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) NASA Langley Research Center Hampton, VA 23665-5225			10. SPONSORING/MONITORING AGENCY REPORT NUMBER NASA CP-10087, Part 1	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) National Aeronautics and Space Administration Washington, DC 20546-0001			11. SUPPLEMENTARY NOTES	
12a. DISTRIBUTION/AVAILABILITY STATEMENT  LIMITED DISTRIBUTION until April 30, 1994 Subject Category 02			12b. DISTRIBUTION CODE	
13. ABSTRACT (Maximum 200 words)  This publication is in four volumes and represents the compilation of papers presented at the First Annual High-Speed Research Workshop held in Williamsburg, Virginia, on May 14-16, 1991. This NASA-sponsored workshop provided a national forum for presenting and discussing important technology issues related to the definition of an economically viable, and environmentally compatible High-Speed Civil Transport. The Workshop and this publication are organized into 13 sessions, with Session 1 presenting NASA and Industry overviews of the High-Speed Civil Transport Program. The remaining sessions are developed around the technical components of NASA's Phase I High-Speed Research Program, which addresses the environmental issues of atmospheric emissions, community noise and sonic boom. Because of the criticality of the materials and structures technology area, and the long-term nature of the supporting research requirements, a session was added in this area to capture the ongoing work at NASA Lewis and NASA Langley and within industry.				
14. SUBJECT TERMS atmospheric science, high lift, laminar flow control, sonic boom, aeroacoustics, supersonic transport, ozone, community noise			15. NUMBER OF PAGES 513	
17. SECURITY CLASSIFICATION OF REPORT Unclassified			16. PRICE CODE	
18. SECURITY CLASSIFICATION OF THIS PAGE Unclassified		19. SECURITY CLASSIFICATION OF ABSTRACT		20. LIMITATION OF ABSTRACT

