Final Report

HALOE Science Investigation
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I. Introduction

This cooperative agreement has investigated a number of spectroscopic problems of interest to the Halogen Occultation Experiment (HALOE). The types of studies performed are in two parts, namely, those that involve the testing and characterization of correlation spectrometers and those that provide basic molecular spectroscopic information. In addition, some solar studies were performed with the calibration data returned by HALOE from orbit.

II. Instrumental Studies

Analysis of data from a gas correlation spectrometer requires considerable knowledge of the characteristics of the spectrometer. All calculations must be performed monochromatically, then the total signal integrated. This ability is required also for some of the testing of the instrument prior to launch. In order to accomplish this a software package was written as part of this cooperative agreement. The HALOE spectroscopic instrument package is a general purpose code that is not designed for sufficient efficiency for final analysis from a gas correlation spectrometer, but provides flexibility for instrumental studies which is far wider than the more efficiently written retrieval software.

The HALOE spectroscopic instrument package was used in various tests of the HALOE flight instrument. These included the spectral response test, the early stages of the gas response test and various spectral response tests of the detectors and optical elements of the instruments.

Considerable effort was also expended upon the proper laboratory setup for many of the prelaunch tests of the HALOE flight instrument, including the spectral response test and the gas response test. These tests provided the calibration and the assurance that the calibration was performed correctly.

III. Spectroscopic Studies

Numerous spectroscopic studies were performed under this cooperative agreement. These studies are documented in the publications listed in section V. Two of the studies are ongoing and these will be published in more detail as they are completed. The studies have all been included or will be included, if appropriate, in the United States Air Force's HITRAN database of spectroscopic line parameters.

Techniques of analysis of experimental spectroscopic data have been given high priority in these studies. The standard least squares spectrum fitting technique was expanded to much larger cases than had ever been tried before and the technique was expanded to the simultaneous analysis of many spectra acquired under different physical conditions and even with different spectrometers. These new techniques are orders of magnitude more rapid than the former techniques and with the rapid increase in speed of computers during this time, projects that were once unimaginable are now routine. In addition, the multispectrum technique makes the detection and measurement of parameters such as line mixing relaxation matrix elements possible for the first time from experimental data.

A very large, detailed study of the carbon dioxide molecule was successfully undertaken. The largest studies were undertaken in the spectral regions of the HALOE NO and CO_2 channels, but the regions studied actually were much broader than these channels. This large number of spectral line identifications, positions and intensities made it possible for Richard Wattson to improve the theoretical model of this molecule. The result has been a large improvement in the CO_2 spectroscopic line parameters available to HALOE in all spectral regions. The study in the region of the HALOE CO_2 channel and the studies of minor isotopomers are ongoing.

The methane molecule was also targeted as one that required better understanding in order to retrieve mixing ratios by way of the HALOE orbital data. Here, the theory upon which the experimental data could be analyzed was much less complete. During the time of this cooperative agreement, there was considerable improvement in the ability to theoretically predict positions and intensities of methane spectral lines by a French group. This enabled us to experimentally measure these same quantities as well as the widths and shifts (and their temperature dependencies) of these spectral lines which have proven too difficult to calculate from theory. The resulting spectral line parameters were disappointing in their ability to reproduce the experimental spectra from which they were derived. Application of Dicke line narrowing to the spectral lines was of no help. Application of line mixing in the Rosenkrantz approximation showed great promise, but further analysis showed that this approximation is not expected to be very accurate in the case of methane in the spectral region of the HALOE HCl and methane channels. A simple theory was applied to calculate the relaxation matrix elements and then exact line mixing theory applied to the calculation of the spectrum. The success of this technique was spectacular when only spectra from a single broadener at a single temperature were included. This theory was used to derive new spectral line parameters for both air and self broadening including temperature dependence for the air broadening. These parameters are the best now available for methane in this spectral region and were incorporated into the version 19 HALOE retrievals.

A number of other studies were undertaken for other reasons. These ranged from assistance in a larger study of ozone which has a large impact upon the HALOE ozone and HCl channels, a study of the temperature dependence of the halfwidths and shifts of methane spectral lines in the spectral region of the HALOE HF channel and various studies of minor isotopomers or spectral regions not used by HALOE which have lesser or no effect on the HALOE retrievals. These latter studies contribute to the overall theory of the molecules in question and improvement in this theory produces improved spectral lines where HALOE needs them.

Spectroscopic efforts under this study also included keeping the HALOE project abreast of relevant studies by other groups concerning newly measured or predicted spectral line parameters.

IV. Solar Studies

Philip Spickler used the HALOE solar scan data to study the surface of the sun for his Ph.D. dissertation. The center to limb brightness function of the quiet sun was measured in the 2.5 to 10 micrometer spectral region to much greater precision than ever before. The relative brightness over the surface of the sun was measured to better than 0.1%. The results of this study along with comparisons to what is predicted by solar atmospheric models is reported in a 1996 Solar Physics article (see section V). The center to limb intensity functions were quite different from those predicted by earlier studies, but that observed was consistent with the current temperature models of the sun.

These solar studies have also been supplemented with similar studies of some sunspots. The results show a considerable variation in the temperature structure of sunspots. This work appears in part in the dissertation and is an ongoing study.

V. Publications

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Absolute Intensity Measurements of CO_2 Bands in the 2395-2680-cm^{-1} Region.
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Curtis P. Rinsland and D. Chris Benner
Applied Optics **23**, 4523 (1984).

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