Validation of SAGE-III Measurements of NO_3: Ground-Based Vertical Profile Measurements

Status Report and Revised Statement of Work
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Goals of the Investigation

The SAGE III Science Team has established requirements for validation studies to assess the precision and accuracy of the SAGE III measurements of O_3, NO_2, H_2O, NO_3, OClO and other trace species. The work described in this report is aimed at providing ground-based vertical profile and column measurements of NO_3 and NO_2 using the same methodology as the actual SAGE III technique, i.e. lunar and solar occultation in the UV/visible spectral region. Spectra are recorded using two different instruments: a 0.05 cm^{-1} interferometer (FTUVS) and a grating spectrograph which utilizes a diode array detector. Both instruments are located at the Table Mountain Facility of the Jet Propulsion Laboratory. Measurements are compared with results from the Caltech/JPL 1-d model to validate mechanisms of stratospheric NO_x chemistry.

At this writing, SAGE III is in orbit and is operating in both solar and lunar occultation modes. Preliminary level 2 data have been generated from data acquired in the lunar occultation mode and vertical profiles of O_3, NO_2 and NO_3 have been obtained. *Validation data are crucially important at this stage of the SAGE III checkout phase.* Within the constraints of the present SAGE III orbit, it will be possible to obtain data at the latitude of Table Mountain Facility during the months of March, April, and July-December during 2002. Our goal is to provide validation data during as many of these opportunities as weather and resources will permit.

Key Accomplishments

Since its inception, this investigation has accomplished several important objectives including:

- Design, construction and deployment of a ground-based UV-visible spectrometer and pointing system for the measurement of trace atmospheric species. The spectrometer has a 1024 channel diode array detector, and operates over the wavelength range 290-1050 nm with a spectral resolution of 0.2 nm. The operating modes include direct solar or lunar absorption, or multi-angle detection of scattered light. The spectrometer is located at JPL's Table Mountain Facility, near Wrightwood, California. A portable spectrometer and pointing system for use in validation measurements for locations other than Table Mountain is currently being designed.
- Acquisition of an extensive database of NO_3 diurnal column abundance measurements. We have conducted NO_3 measurements on 52 nights near full moon beginning in June, 1999. Each night we recorded as many as 25 spectra from which NO_3 column abundance measurements can be retrieved.
- Development of algorithms for retrieval of NO_3 column abundance measurements from lunar spectra. Two different algorithms have been developed and are currently being

intercompared. One algorithm uses a direct fit approach while the other uses the DOAS (differential optical absorption spectroscopy) approach.

Progress Since August, 2001

Algorithm Development

As discussed in previous reports, processing of lunar spectra to obtain the NO_3 column abundance consists of several steps including dark noise subtraction, wavelength calibration using line spectra from a neon emission lamp, ratioing of the spectra with a reference spectrum taken before appreciable buildup of NO_3, and fitting of the resulting absorption spectra using reference spectra for NO_3 and other species including H_2O, O_2, O_3, etc.

In previous reports we have outlined the development and presented results obtained using a spectral fitting code developed within our group. While this code has worked satisfactorily, it lacks the ability to perform iterative non-linear optimization in the wavelength domain. This feature is important because it permits the code to correct for small temperature-dependent drifts in the spectrometer that affect both the wavelength calibration and dispersion. Rather than augment our existing code, we have acquired a new code called "MFC", developed over a period of years by the group of Prof. Ulrich Platt at the University of Heidelberg [Stutz and Platt, 1996].[1] MFC is an extremely powerful code which has been tested in both laboratory and field applications. Its main operational modes include: manual and automatic acquisition of spectra, analysis of weak absorption bands by various numerical techniques including filtering and fitting, and storage and retrieval of spectra. The program runs in both MS-DOS and UNIX environments, and is actively supported by the Heidelberg group. We have established a collaboration with Prof. Jochen Stutz of the Department of Atmospheric Sciences, UCLA, who is one of the principal co-authors of the code. With the assistance of Prof. Stutz and his student, we have successfully retrieved NO_3 column abundances from several of our lunar spectra. Our preliminary assessment indicates that the nonlinear fitting approach used in MFC will improve the quality of our retrievals. Further evaluation is necessary before a decision is made concerning the choice of an operational code.

Measurements of NO_3

With the current approach, NO_3 spectra are obtained using the Moon as a light source when the lunar phase is within two days of full. This requirement arises both from the sharp dependence of lunar intensity on lunar phase, and from the need to match the temporal dependence of NO_3 with the availability of the Moon as a target. The number of viewing opportunities is further limited by clouds. Since the last progress report (August, 2001), good lunar spectra were obtained during the full moon periods of the months of December, 2001, January 2002 and February, 2002. Measurements for the full moon period of March, 2002 will be carried out as well.

Instrument Development

As indicated in previous progress reports, instrument development activities are also underway that are aimed at increasing the quantity and quality of evaluation data. These include improved temperature control and stabilization of the spectrometer, evaluation of commercial

[1] Stutz, J. and Platt, U.,Appl. Optics, **35**, 6041-6053 (1996).

CCD cameras to replace the existing diode array camera, and automation of the data acquisition process. Progress is being made in all three areas.

Planned Activities

The activities for the coming year may be summarized as follows:

NO_3 Measurements

1. NO_3 measurements will be carried out at every full moon viewing opportunity, weather permitting.
2. Coordinate plans for validation measurements with the SAGE III Science Team. Discussions are underway with W. Chu and C. Trepte of LARC for exchange of spectra obtained from SAGE III and our ground-based spectrometer. This intercomparison of spectra should be extremely useful to both teams.
3. Continue the evaluation of the retrieval code "MFC" for the analysis of ground-based NO_3 spectra.

Modeling

1. The JPL/Caltech one-dimensional atmospheric model will be used in the analysis of NO_2 and NO_3 measurements from FTUVS and the spectrograph. Comparisons will be made between measurements and model calculations of the NO_3 column constrained by measurements of NO_2 from the spectrograph, the O_3 vmr from the DIAL system at TMF, NCEP temperature profiles and other relevant trace species measurements from UARS and other spacecraft. The results will be used to assess the adequacy of existing models of stratospheric NO_x chemistry.

Schedule

Tasks are referenced to the numerical levels in the previous paragraphs

Task/ Month	*Mar 2002*	*Apr*	*May*	*Jun*	*Jul*	*Aug*	*Sept*
NO_3							
1							
2							
3							
Models							
1							

Collaboration with the SAGE III Instrument Team:

There are several areas of mutual interest between our group and the SAGE III Instrument Team including:

- comparison of retrieval algorithms for NO_3 and other species using lunar spectra
- treatment of interfering spectral features
- use of a common spectroscopic database for NO_3 and other molecules
- methods for the comparison of SAGE III vertical profiles with the column and profile data obtained from ground-based sensors

- separation of the NO_3 contributions from the stratosphere and troposphere, especially where regional NO_x sources are important

The PI of this task will attend SAGE III Science Team meetings if invited by the SAGE PI.

Exchange of Correlative Data with Instrument Team and Other Investigators: It is our intention to disseminate the correlative data from this investigation to the Instrument Team as quickly as possible. While a protocol for this exchange has not yet been established, this will be accomplished well in advance of the SAGE III launch. Data from the correlative measurements will be available on our ftp site for rapid dissemination to interested users.

Budget (FY02, April-Sept.)

The previous report requested support for this task covering the first six months of FY02. The current request encompasses the second half of FY02. Resources are requested for 0.5 WY of a JPL/Caltech postdoctoral fellow (Dr. Claudine Chen), who is responsible for data acquisition and data analysiss and approximately 2 months of support for Dr. Richard Cageao (JPL science staff) who supports the instrument development and data acquisition activities.

Direct Compensation		
Dr. Claudine Chen (JPL Postdoc)	883 workhours	$19.8 K
Dr. Richard Cageao	346 workhours	$15.0 K
Benefits (49.3%)		$17.2 K
TOTAL		$52.0. K