PARTICIPATION IN THE TOMS SCIENCE TEAM

NASA Grant NAG5-7489

Final Report
For the period 1 June 1998 through 31 May 2002

Principal Investigator
Dr. Kelly Chance

September 2002

Prepared for
National Aeronautics and Space Administration
Washington, DC 20546

SMITHSONIAN INSTITUTION
ASTROPHYSICAL OBSERVATORY
CAMBRIDGE, MASSACHUSETTS 02138

Director: Irwin I. Shapiro

The Smithsonian Astrophysical Observatory is a member of the Harvard-Smithsonian Center for Astrophysics

The NASA Technical Officer for this grant is Ernest Hilsenrath 916.0, NASA/GSFC Greenbelt, MD 20771
Smithsonian Astrophysical Observatory
TOMS Science Team Participation
Final Report

Principal Investigator
Dr. Kelly Chance
Smithsonian Astrophysical Observatory
Atomic and Molecular Physics Division

Because of the nominal funding provided by this grant, some of the relevant research is partially funded by other sources. Research performed for this funding period included the following items:

- We have investigated errors in TOMS ozone measurements caused by the uncertainty in wavelength calibration, coupled with the ozone cross sections in the Huggins bands and their temperature dependence. Preliminary results show that 0.1 nm uncertainty in TOMS wavelength calibration at the ozone active wavelengths corresponds to ~1% systematic error in \( \text{O}_3 \), and thus potential 1% biases among ozone trends from the various TOMS instruments. This conclusion will be revised for absolute \( \text{O}_3 \) measurements as cross sections are further investigated for inclusion in the HITRAN database at the SAO, but the potential for relative errors remains.

- In order to aid further comparisons among TOMS and GOME ozone measurements, we have implemented our method of direct fitting of GOME radiances (BOAS) for \( \text{O}_3 \), and now obtain the best fitting precision to date for GOME \( \text{O}_3 \) columns. This will aid in future comparisons of the actual quantities measured and fitted for the two instrument types.

- We have made comparisons between GOME ICFA cloud fraction and cloud fraction determined from GOME data using the Ring effect in the Ca II lines. There is a strong correlation, as expected, but there are substantial systematic biases between the determinations. This study will be refined in the near future using the recently-developed GOME Cloud Retrieval Algorithm (GOMECAT).

- We have improved the SAO Ring effect determination to include better convolution with instrument transfer functions and inclusion of interferences by atmospheric absorbers (e.g., \( \text{O}_3 \)). This has been made available to the general community.
• Attended TOMS Science Team meeting in Huntsville, AL, May 2000. Gave talk "TOMS lessons from GOME and GOME lessons from TOMS."

• Investigated wavelength calibration errors in the Bass-Paur ozone cross sections by correlation with FTS measurements performed at the University of Bremen (J. Orphal, private communication, 2000). The results are that: (1) The cross sections are in error by an overall wavelength correction of 0.015±0.040 nm. Slightly different results, with smaller error bars, can be obtained by fitting only over narrower ranges in the Huggins bands (e.g., 324-343 nm), but such results are not consistent over the entire Bass-Paur spectral range. (2) The error in absolute ozone corresponding to this uncertainty is 0.4%. (3) For TOMS and for the other satellite-based ozone monitoring instruments, it is necessary to have new, FTS-based measurements of the ozone cross sections, including their temperature dependences through the Hartley-Huggins and Chappuis bands (the latter because future satellite-based instruments will need to be able to combine UV and visible O₃ measurements).

• Created improved solar reference spectrum from 235 to 1100 nm at 0.01 nm resolution by combining lower resolution solar spectra with good absolute intensity calibration: SOLSTICE/SUSIM spectra from UARS (shorter wavelength range) and the LOWTRAN/MODTRAN reference spectrum (longer wavelength range), merged together over 405.6-410.6 nm, with a high resolution ground-based solar spectrum [R.L. Kurucz, I. Furenlid, J. Brault, and L. Testerman, Solar Flux Atlas from 296 to 1300 nm, National Solar Observatory, Sunspot, New Mexico, 240 pp., 1984; K. Chance and R.J.D. Spurr, Ring Effect Studies: Rayleigh Scattering, Including Molecular Parameters for Rotational Raman Scattering, and the Fraunhofer Spectrum, Applied Optics 36, 5224-5230, 1997]. This spectrum is supplied with a computer program for convolution to a selected spectral resolution. It has been made available to the general atmospheric measurement community.

• Due to the gap in effective ozone measuring capability caused by problems with Earth Probe TOMS, later exacerbated by QuikTOMS launch failure, we began a program of fitting GOME spectra for total O₃ column using our best spectral fitting procedure and the wavelength-corrected Bass-Paur ozone cross sections. This procedure fits to the slant column O₃ followed by determination of vertical column ozone using air mass factors calculated with the SAO LIDORT radiative transfer code.

• We have since developed a method for direct fitting of GOME spectra to determine vertical columns by including the radiative transfer modeling in the fitting procedure. The procedure includes the adjustment of ozone profile shapes for geolocation, time, and the total ozone column by interpolation to the TOMS Version 8 ozone profile climatology. The
procedure is currently in the process of being implemented and will be fully tested in the coming year.