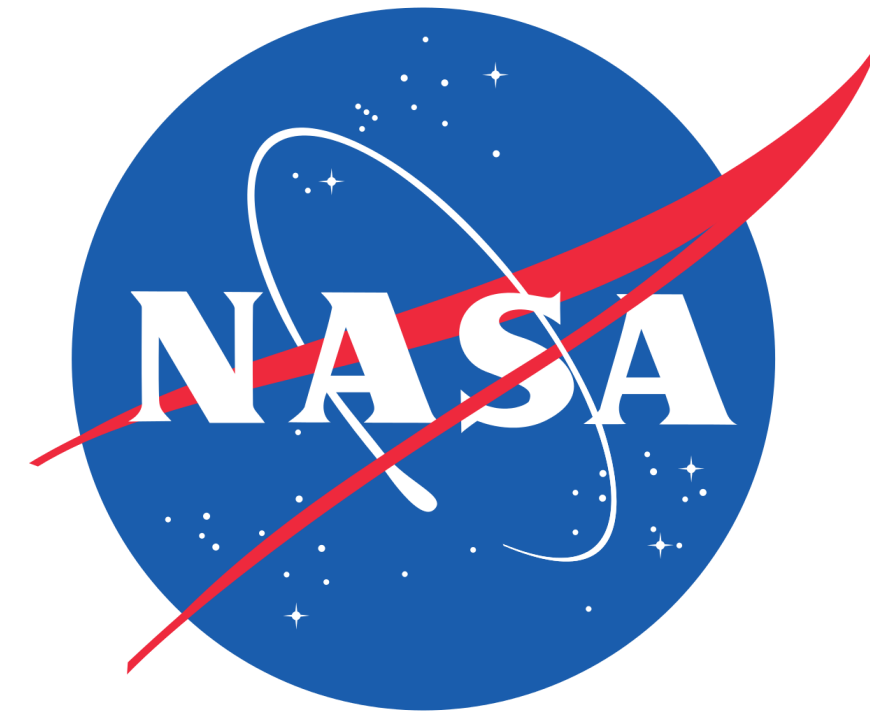




An initial evaluation of ozone data quality from SAGE III/ISS v5.1

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Abstract

The Stratospheric Aerosol and Gas Experiment (SAGE) III is a solar occultation instrument installed on the International Space Station (ISS) that has been providing vertically resolved measurements of aerosol extinction, ozone concentrations, and other trace gases. With a legacy going back to the late 1970s, SAGE ozone measurements have been a vital contributor to international ozone assessments and analyses on stratospheric ozone trends. As the newest SAGE instrument, SAGE III/ISS will continue to provide high precision profiles of ozone that will help determine if the Montreal Protocol has been successful in enabling the recovery of the ozone layer. However, as is a necessary step for all new instruments, a rigorous validation of the data quality is required to determine if the data is sufficient for incorporation into trend analyses. Herein we discuss an initial evaluation of the data quality of vertical profiles of ozone with a focus on internal consistency for the first validation version (v5.1) derived from SAGE III/ISS measurements.

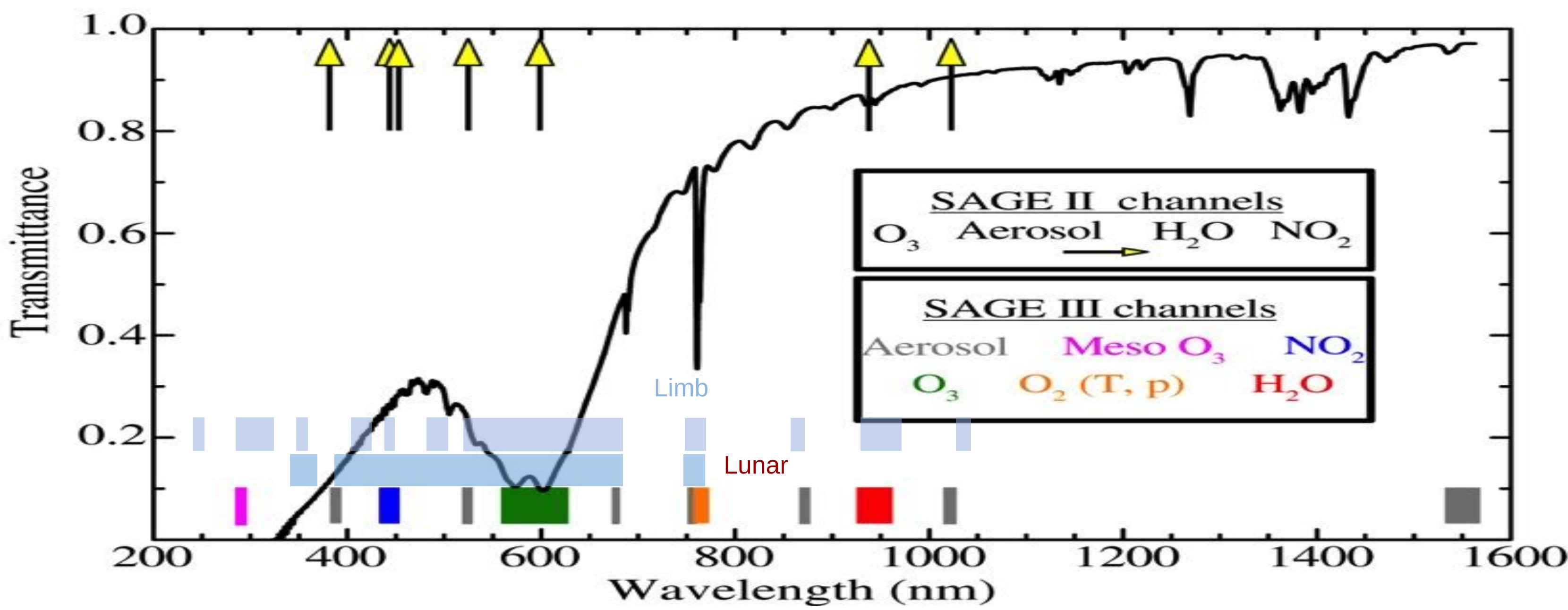
References

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SAGE III/ISS Ozone Products

SAGE III/ISS utilizes a CCD spectrometer and makes multispectral measurements of the solar disk above and through Earth's limb to create vertical profiles of line-of-sight transmission at each wavelength. This information is then processed through an inversion algorithm to produce vertical profiles of constituent species. As it pertains to ozone, SAGE III actually produces three separate products. The first two both use ozone absorption in the Chappius band (near 600 nm) to retrieve vertical profiles of ozone up to 70 km. One is a narrow-band retrieval dubbed "O3_MLR" while the other is a broadband retrieval dubbed "O3_AO3" that is most similar to the earlier SAGE II instrument (1984-2005). The third retrieval dubbed "O3_MES" uses absorption features in the ultraviolet (<300 nm) to retrieve vertical profiles between ~45 and ~100 km.

The figure below illustrates the spectral sampling regions utilized by SAGE III/ISS. For comparison, the seven channels used by SAGE II are denoted by yellow arrows while the spectral regions (with resolutions as small as ~1 nm) used by SAGE III/ISS solar occultation measurements are shown at the bottom and colored (where specific) by species. SAGE III/ISS can also operate in a lunar occultation mode and a limb scatter mode. Those spectral sampling regimes are also illustrated but are not a focus here.



Known Anomalies in Version 5.1

The retrieval algorithm for SAGE III/ISS is, for all intents and purposes, the same as that used for SAGE III/M3M (2002-2006). However, while many improvements have been made to the SAGE II dataset over the years, SAGE III/M3M (and thus SAGE III/ISS) has not benefited from those changes. We intend to spend more attention to the details of the SAGE III/ISS retrieval algorithm to determine what lessons learned from the SAGE II v7.0 algorithm (Damadeo et al., 2013) can / should be incorporated.

The SAGE III/ISS instrument is by far the most / best characterized SAGE instrument. The detailed knowledge of the intricacies of the instrument's behavior and performance offer us the ability to incorporate several new algorithms to improve the data quality. One such characterization is that of the spectral stray light within the CCD (reentrance spectra). While still on the ground, a thorough characterization of the spectral stray light was performed on the instrument and one particular problem area was identified. A portion of the light incident on the UV range of the CCD actually comes from near the peak of Chappius ozone absorption. This will have a negative impact on the mesospheric ozone retrieval and needs to be corrected for. While a rudimentary correction is currently implemented, it stems from a similar theoretical analysis on the SAGE III/M3M instrument and does not use the most up-to-date information. As such, we do not recommend the MES product for validation studies as it is likely biased.

The SAGE III/ISS algorithm makes use of an external climatological data set (MERRA2) for temperature and pressure data, which is necessary for modeling refraction and molecular (Rayleigh) scattering. These data are provided with geopotential heights, which the algorithm converts to geometric altitudes at the location of the measurement. It has been discovered that this conversion between geopotential height and geometric altitude, which was actually copied from the SAGE II v7.0 algorithm, was never thoroughly vetted and is more of an approximation. As such, the current altitude registration of the meteorological products are biased on the order of 100 or so meters (altitude and latitude dependent) as shown on the left. The impact of this mis-registration would be most noticeable when converting to mixing ratio on pressure space. It is, of course, also noteworthy to point out that, since the code was present in the SAGE II v7.0 algorithm, that data product has a similar bias.

Since aerosol measurements are intertwined with ozone measurements, assessing the quality of the aerosol product can also yield information about the quality of the ozone product. In SAGE III/ISS, the aerosol product derives from the MLR algorithm, meaning it is not solved for directly but rather is treated as a residual after solving for O3 and NO2 and removing their influences (along with Rayleigh scattering). The figure at left and bottom shows all of the aerosol extinctions in the tropics at 16 km for each of 8 spectral channels in blue, and the medians of these values in red. Physically, this "aerosol spectrum" should be slowly varying and monotonic but instead exhibits a "dip" near 600 nm that tends to be larger at lower altitudes. Since this is the primary location of ozone absorption, it is possible that this negative aerosol anomaly corresponds to a positive ozone anomaly in the MLR product.

Assessment of O₃ Data Quality

Since this is meant to be more of an internal look at the SAGE III/ISS ozone products (there are several presentations at this workshop on inter-instrument comparisons), there is only so much that can be investigated. The obvious first things to look at such as expected seasonal variability or correlations between species (e.g., positive correlations between NO₂ and O₃ in the Antarctic polar vortex) reveal nothing out of the ordinary (not shown here). Another thing that can be investigated is the behavior of the reported uncertainties. In general, uncertainties are higher at lower mixing ratios or in the presence of elevated aerosol loading as expected (shown at left). What is interesting is how the AO3 uncertainties (blue) are systematically smaller than those of the MLR product (red). They also exhibit an increased range. We note that this is worth investigating to ensure that reported uncertainties are reasonable so that they can be utilized in scientific studies.

Since the retrieval algorithm currently produces two ozone products in the stratosphere, it is not unreasonable to ask which is the better product. By utilizing the residual analysis detailed in Damadeo et al. (2014), we can get an independent assessment (i.e., independent of any other data set) of just that. Using a simple regression to only SAGE III/ISS data, we can see (right, top panels) that the spread of the uncorrelated residuals is similar throughout most of the stratosphere between the two products. However, the MLR product is significantly noisier than the AO3 product both in the upper-most stratosphere and mesosphere as well as in the lowermost stratosphere and troposphere. These results are similar to those from a study (Wang et al., 2006) of SAGE III/M3M data using comparisons with other data sets. Since studies often investigate data in these ranges, we recommend that the AO3 product be used.

As an occultation measurement that makes measurements at only two distinct times of day (sunrise [SR] and sunset [SS]), comparing SRs and SSs offers another opportunity to assess data quality and diagnose potential anomalies. The contour plots at right show the perceived diurnal variability (i.e., differences between SR and SS events) from the regression (stippling denotes regions that are not statistically significant at the 2-sigma level). Since the MLR product is inherently noisier, so too is its SR/SS differences. Still, the pattern of diurnal variability in the tropics is similar to that seen in SAGE II (far right), which is itself too large. This may indicate that the enhanced diurnal variability in SAGE III/ISS has a similar root cause to that of SAGE II, which we have reason to believe may be algorithm related.

