SAGE III on ISS Version 6.0 Release Notes

This statement applies to SAGE III/ISS Version 6.0 (Solar Level 1B, Solar Level 2, and Lunar Level 2) data products.

Reader Software:

Both IDL and Python reader software are available to access the products in the native format. New readers are required for this release. The product formats have changed significantly, so new readers are being provided. However, readers for previous versions of SAGE III data are not compatible with this version and the new version of the IDL and Python data readers are not backwards compatible with the previous version of the data product. The Python readers provide both a new and legacy naming convention in an effort to limit the impact on users' existing analysis code.

General Comments:

This release contains the fifth official release of SAGE III/ISS products that are suitable for use in both validation and research studies for some data products (see the Data Product User's Guide for details). Version 6.0 replaces Version 5.3 and the public are invited to continue to make comments on the new release.

Vertical profiles of ozone (O_3), nitrogen dioxide (NO_2), and water vapor (H_2O) concentrations as well as multi-wavelength aerosol extinction coefficient and derived aerosol products are included in the solar Level 2 data product files. Three ozone profiles are available in this release of the solar products: a UV-based mesospheric product (i.e., "o3_mes" in the product files) and two Chappuis-based products. One Chappuis-based product uses a spectrally focused spectral fitting retrieval (i.e., "o3_mlr") while the other uses a broad-spectrum retrieval scheme that is similar to that of SAGE II (i.e., "o3_ao3"). A blended/composite ozone product and retrieved temperature/pressure products are not included in the v6.0 data set. To make things easier for the user, v6.0 now includes a generic "o3" product, which is the currently recommended ozone product to use for research purposes (currently just a copy of the o3_ao3 product). Vertical profiles of ozone, nitrogen dioxide, and nitrogen trioxide (NO_3) concentrations are included in the lunar Level 2 product files. Chlorine Dioxide (OClO) from lunar occultation are not included in this release. The channel wavelengths used in solar and lunar retrievals are available in the Data Product User's Guide (DPUG).

Loss of Events

The mid-inclination orbit of the ISS periodically results in high solar beta angles ($|\beta|>60°$) that make solar occultation measurements impractical. Additionally, events are occasionally not acquired due to obstructions of the Sun or Moon by the ISS or its components. There are brief periods during which SAGE III measurements are not taken due to unfavorable ISS configuration or activities (e.g., abnormal orientation, Extravehicular Activity (EVA), or 'new' space vehicle arrival). A space vehicle of one kind or another is always docked at the ISS and generally presents no harm to SAGE III.

A number of other special cases occur with varying frequency and may affect data quality. These include situations where 1) the pointing system (hexapod) was unable to move the instrument into the requested position for the event, 2) the contamination window was closed for the event, 3) the ISS time correction parameter was invalid, but could be corrected by interpolation, 4) large mechanical vibrations occurred, 5) a line-of-sight, structural blockage was detected and mitigated during the exoatmospheric portion of the event, 6) spectral calibration could not be performed (likely due to a blockage), 7) a solar eclipse occurred during a portion of the event, 8) the scan head pointing drifts more than 1 degree off-nadir during an event, and/or 9) disturbance correction skipped. Such cases are indicated by boolean data products.

Broad Changes from v5.3 to v6.0:

As is common with any new version of data, there are a long list of minor changes and bug fixes, but there are also a few significant changes that broadly affect the data products. Those significant changes are listed here, as are any minor changes or bug fixes that address known anomalies in the data. Minor changes or bug fixes that do not have a noticeable impact on the data products are not discussed. Changes specific to an individual product are detailed in the Solar or Lunar product notes later.

Filling Transmission Gaps

Unlike previous SAGE instruments, operating from ISS presents the unique challenge of having occasional obstructions in the field of view (i.e., other parts of ISS). These obstructions can cause a gap in the observation at a particular altitude. Additionally, during periods of high solar activity, numerous and large sunspots may occupy a significant portion of the overall solar limb darkening curve. Since data within sunspots are excluded from the transmission profile, an excessive number of excluded data packets can cause gaps. This is true even with multiple successive scans spanning a particular altitude as the altitude registration of multiple sunspots will sometimes align. Because the processing from Level 1 transmission to Level 2 vertical species profiles requires a continuous transmission profile, we have allowed the interpolation of transmission data across small gaps (i.e., no larger than 3 bins or 1.5 km). We have also inserted a flag in each vertical bin to state whether it comes from interpolation of adjacent bins or was measured.

L1 Uncertainty Improvement

As was done for the version 7.0 SAGE II algorithm, we have incorporated a component in the uncertainty that stems from the uncertainty in the exoatmospheric solar scans as they propagate through the algorithm. As this is an additional component of uncertainty, it increases the overall uncertainty budget in the transmission profiles. This is most influential at the tops of profiles and reduces lower in the atmosphere. The magnitude also varies with wavelength, as some of the pixel groups on the detector are aggregated prior to being read off, but it can be as large as 25% of the v5.3 L1 uncertainties in the exoatmospheric regime. Practically speaking, this can lead to increases in L2 uncertainties on the order of 5–20% of the v5.3 uncertainties (e.g., a change from 2.0% to 2.4% relative uncertainty) in the middle to upper stratosphere.

Change of O3 Absorption Cross-sections

Motivated both by a change in the community standard and an apparent deficiency in retrieved aerosol extinctions near the peak of the O3 Chappuis absorption band as discussed in the literature, we have changed the O3 cross-section database used in the retrieval algorithm from the SCIAMACHY V3 database (Bogumil et al., DOI:10.1016/S1010-6030(03)00062-5, 2003) to the Serdyuchenko-Ghorshelev database (Serdyuchenko et al. [Data set], DOI:10.5281/ZENODO.5793206, 2014). This results in a roughly 2% increase to O3 concentrations that does vary slightly with altitude because the cross-section changes are temperature dependent. However, this change significantly mitigates the negative bias that can be seen in the aerosol extinction spectrum near the Chappuis that was a non-physical result of incorrect spectroscopy.

Solar Product Changes:
Aside from the differences associated with the change in O3 cross-section database, there are minimal changes to the solar products from v5.3 to v6.0.

Covariance in Aerosol Uncertainties
We have improved the robustness of the statistical computation of uncertainty in the L2 aerosol profiles for aerosol channels 2 (~449 nm) and 8 (~1 μm). While each aerosol channel covers multiple pixel columns on the detector, some are aggregated prior to being read out and others are aggregated after. Channels 2 and 8 are in the latter category, which means the separate pixel groups are highly correlated. We now consider the covariance of these pixel groups when computing the uncertainty in these aerosol products, which naturally increases the uncertainties by up to 5% relative uncertainty.

Incorporate Aerosol Flags and PSD Information
In keeping with part of the intent of the independently funded NASA ROSES Science Team, we have incorporated results from some of that research into the SAGE III/ISS data products, specifically additional products derived from the aerosol extinction data. The first is a flag that indicates if the aerosol extinction value in the file is associated with background, elevated aerosol, or cloud (for each wavelength and altitude) (see Kovilakam et al., DOI: 10.5194/amt-16-2709-2023, 2023 for details). The second is a collection of derived parameters associated with the particle size distribution (for each altitude) (see Knepp et al., DOI: 10.5194/amt-17-2025-2024, 2024 for details). These derived data products were independently hosted for download at NASA but are now being incorporated into the SAGE III/ISS data files. Please see the SAGE III/ISS Data Product User's Guide for additional details.

Lunar Product Changes:
No significant changes specific to individual Level 2 data products have been implemented.