SAGE III on ISS Version 5.3 Release Notes

This statement applies to SAGE III/ISS Version 5.3 (Solar Level 1B, Solar Level 2, and Lunar Level 2) data products.

Patch Notes

When necessary, SAGE III/ISS software may be updated to address unexpected problems, or "bugs". As long as the bug fixes would not alter already-released products, they may be added as a "patch" to the version in production. These Release Notes provide information on the content of each patch.

Patch 1 (September 2023)

- On 3 August 2023 one of three ring laser gyroscope axes for the Disturbance Monitoring Package ceased generating reliable data (see the **DMP Correction** section below for more information on these data). The axis measured disturbances in the instrument's azimuthal direction, which is inconsequential to scan plane disturbances. Data from that axis are permanently removed from the pointing correction starting with the events of that date. This removal was assessed and found to have no signification impact on the DMP Correction.
- Python reader software is updated to accommodate the deprecation of some data type aliases (*numpy.int* and *numpy.float*) as of NumPy 1.20.0. The types *numpy.int32* and *numpy.float32* are now used instead.

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 slightly, so new readers are being provided. Readers for previous versions of SAGE III data are not compatible with this version. However, the new version of the IDL and Python data readers are backwards compatible with the previous version of the data product. Note that Version 5.3 product files in HDF format are not supported by the readers, though v5.1 HDF files are still supported.

General Comments:

This release contains the fourth 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 5.3 replaces Version 5.2 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 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., "Ozone_Mes" in the product files) and two Chappuis-based products. One Chappuis-based product uses a spectrally focused spectral fitting retrieval (i.e., "Ozone_MLR") while the other uses a broad-spectrum retrieval scheme that is similar to that of SAGE II (i.e., "Ozone_AO3"). Composite ozone and retrieved temperature/pressure products are

not included in the v5.3 data set. Vertical profiles of ozone (O_3), nitrogen dioxide (NO_2), 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 in the product files by the issuance of a bit flag.

Broad Changes from v5.2 to v5.3:
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.

DMP Correction
SAGE III/ISS is an occultation instrument that retrieves vertical profiles of aerosol extinction coefficients, ozone, water vapor, and other trace gas concentrations. The nature of the occultation technique used by the SAGE series of instruments requires accurate and precise pointing knowledge. On a spacecraft with a relatively benign mechanical vibration environment, like the Earth Radiation Budget Satellite, the developed methodology performs superbly, allowing the retrieval of precise ozone profiles from SAGE II observations. However, operating on the ISS poses challenges, as it is frequently visited by vehicles, performs maneuvers, and experiences other mechanical disturbances that affect the pointing of the instrument during measurements. A Disturbance Monitoring Package (DMP) comprised of a miniature inertial measurement unit built by Honeywell Aerospace that measures rotation in inertial space using ring laser gyroscopes oriented about three orthogonal axes is used to improve the pointing knowledge. The

data from the DMP have been incorporated into the science processing algorithm to correct pointing errors caused by these mechanical disturbances.

The DMP correction has been determined to improve pointing accuracy in general and is applied to all observations unless DMP data are unavailable, and a DMP usage flag notifies users. DMP flags are included in the product files to indicate disturbances where pointing errors prior to correction exceeded mission requirements. The DMP corrections are only applied to the solar products and are not implemented for Lunar products at this time.

72 Layer MERRA-2 Input and Other Meteorological Data Changes
There were a few changes to the meteorological inputs used for v5.3 processing. The most significant of these changes was moving to 72 layer MERRA-2 data from the 42 level MERRA-2 data used in previous versions. The 72 layer MERRA-2 data, unlike the 42 level MERRA-2 data, doesn't have data at constant pressure levels so the pressure is now interpolated. Other changes include a bug fix to include the previously neglected uppermost level of MERRA-2 data, and a process change to accommodate reprocessed MERRA-2 data. These changes to the meteorological data produced no significant differences below the mesosphere.

Bottom of Transmission Profile Interpolation Fix
For profiles with one or two data packets for interpolation of the transmission bin, the least squares fit in the processing algorithm was being used incorrectly. This was corrected in v5.3 by changing the criteria for interpolation. For bins with more than two data packets, a least squares fit is still performed, while a linear interpolation is used for bins with two data packets, and bins with one data packet default to that value.

Flag Restoration and Fixes
We have restored some broken flags within the product files and updated the definitions for the flags. The product QA flags have been restored after being removed in v5.2. Since smoothing of the products is still turned off the QA flags are only set if needed for bits 4-5. These bits are set for: retrieved slant-path profile value was negative, retrieved slant-path profile value contained 'fill' data. The ephemeris quality flag was restored and given new definition of missing, nominal, expanded interpolation time window, or time gap/bad data. Further, a bit indicating scan head pointing drift of more than 1 degree off-nadir was added to the event condition QA flag.

Ephemeris Interpolation Fix
Prior to v5.3 the ephemeris interpolation was failing for events where there were not enough data points to perform the interpolation causing a crash and loss of the entire day's events. The fix was to expand the window of interpolation for these events to get enough data for interpolation allowing the day's events to be recovered.

Solar Product Changes:
The automated QA filtering of events was modified. For v5.3, the auto QA has been adjusted to recover events around the Hunga Tonga eruption that were withheld due to auto QA in v5.2. These events were being filtered out due to a flag in the auto QA where "AO3" and "MLR"

differ around the ozone maximum greater than a certain threshold. These events were reviewed, deemed to be releasable, and this auto QA threshold was disabled.

There are minimal changes to the solar products from v5.2 to v5.3. The most notable changes seen in the products is a decrease in reported uncertainty, which results in a decrease in the noise-dominated top of the profiles as the noise floor is lowered.

No significant changes specific to individual Level 2 data products have been implemented.

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