Release Notes for Solar Orbiter SWA Heavy Ion Sensor Level 3 Data V02

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1 Synopsis

This document adds usage notes for the Heavy Ion Sensor (HIS), part of the Solar Orbiter SWA instrument suite. The HIS data are described in detail in the SWA Data Product Description Document (DPDD). This document pertains to only the HIS Level 3 (L3) data, which are the main solar wind composition dataset for the HIS sensor. This L3 designation is in contrast to most other Solar Orbiter instruments, where the main science data is Level 2. HIS can measure over 75 ions in the solar wind over a single energy scan. Additional processing beyond that required for Level 2 data products is needed to accurately assign the raw instrument counts to specific ion species, thus leading to the designation as L3 data.

2 Release and Usage Note

2.1 Changes from V01

The L3 V02 processing of the HIS data refines species separation, improves uncertainty estimation, corrects for additional instrumental constraints on moments calculation, and updates quality filtering. Each of these are further described below.

As a result of these improvements to the data processing, the extended iron charge state distribution and the average iron charge state are available in V02. Furthermore, these changes have allowed for the processing of additional UTC days from 2022-2023.

2.2 Dataset Contents

This data release contains the following subset of data products specified in the DPDD each at nominal 10-min resolution (**bold indicates new or changed data products compared to V01**):

- Elemental Abundances: Sums of densities for all charge states for two elements, expressed as their ratio
    - Fe/O
- Ionic Charge State Information: Density ratios for specified ion pairs or average charge state, computed as density-weighted average
    - O7+/O6+, C6+/C5+, C6+/C4+

    - $\langle Q_O \rangle$, $\langle Q_C \rangle$, $\mathbf{\langle Q_{Fe} \rangle}$
- Ionic Charge State Distributions: Normalized distribution of all charge states analyzed for specified element (relative abundances of individual charge states sum to 1).
    - Carbon (4-6+), Oxygen (5-8+), and **Iron (6-20+)**
- Kinetic properties: Moments of velocity distribution functions for specified ions.
    - O6+ bulk and thermal speeds in km/s

The above data products are a subset of the data products expected to be ultimately delivered from HIS and as detailed in Owen et al. [2020]. Work is ongoing to release data products for additional ions and elements as they are validated.

2.3 Ion species separation

Attributing HIS measurements to specific ions is done via a maximum likelihood estimator (MLE) process (see Livi et al. [2023] and references therein for details). This approach uses probability density functions (PDFs) of count sources to attribute observations to specific ions. HIS L3 V01 processing used PDFs for all charge states of ten elements: H, He, C, N, O, Ne, Mg, Si, S, and Fe. In V02, additional PDFs are introduced: PDFs representing noise sources (such as time-of-flight accidentals) and PDFs for all charge states of Ca. With the increased total volume of HIS data available since the initial V01 processing, all ion PDFs have been updated in V02 to more accurately match HIS measurements. In particular, these updates to the MLE PDFs refine the species separation of C from He and Fe from Si/S/Ca.

2.4 Moments calculation

HIS L3 V02 calculates moments (density, bulk speed, and thermal speed) via numerical integration of 1D velocity distribution functions (VDFs) in the instrument frame. These are expressed analytically as:

$$n = \sum_i \mathcal{Q}_i f_i v_i^2 \Delta v_i$$

$$u = \frac{1}{n} \sum_i \mathcal{Q}_i f_i v_i^3 \Delta v_i$$

$$v_{th} = \sqrt{\frac{2}{n} \sum_i \mathcal{Q}_i f_i (v_i - u)^2 v_i^2 \Delta v_i}$$

where i is the energy-per-charge (E/q) step, n is density, u is bulk speed, v_{th} is thermal speed, f is phase space density, v is the ion's speed (converted from E/q), Δv is the width of the speed range (converted from the E/q stepping), and $\mathcal{Q}$ is a Boolean operator denoting the validity of the measurements (1 = valid; 0 = invalid). The value of $\mathcal{Q}_i$ is determined by several factors: the E/q steps at which proton avoidance triggered during the data accumulation; if v_i is below the velocity filter used to limit the impact of time-of-flight accidentals; the amount of accumulated

data; and the fraction of the ion's probability density function available for species separation. The value of Q_i can be different for different ions at the same E/q step. For L3 data products that involve only one ion species (e.g., O6+ bulk speed), all $Q_i = 1$ steps contribute to the moment calculation. For data products that involve multiple ion species (e.g., O7+/O6+ charge state ratio), only the common speed range across which $Q_i = 1$ for all species involved in the data product is used to calculate moments. For example, if $Q_i = 1$ for O6+ over 200-2000 km/s but $Q_i = 1$ for O7+ over 100-1500 km/s then Q_i will be adjusted for both species such that $Q_i = 1$ for 200-1500 km/s when calculating the O7+/O6+ charge state ratio.

The definition of thermal speed used in HIS L3 V02 is consistent with $v_{th} = \sqrt{2k_bT/m}$ where T is temperature, k_b is Boltzmann's constant, and m is the ion's mass.

2.5 Data uncertainties

In V02, uncertainties reflect counting statistics as well as uncertainty from species separation. Uncertainties for each HIS L3 data product are provided. In V01, these represented only counting statistics. V02 also incorporates uncertainty associated with the MLE species separation. For each application of MLE to the HIS data, the input PDFs are perturbed via a Monte Carlo process to generate a distribution of solutions. The data products are calculated from the unperturbed solution while the standard deviation across the distribution of solutions is used to quantify the uncertainty associated with the MLE process. While systematic uncertainties may still be present in the data, the reported uncertainties provide a much more realistic estimate compared to V01. **All analyses using HIS L3 data should examine uncertainties of the data products of interest.**

2.6 Quality filtering

V02 uses an updated quality filtering scheme compared to V01. This release uses three quality values: 0 indicates good quality data; 1 indicates potential quality issues but is not clearly of low quality; 2 indicates data that has been filled due to its quality. The record-level quality flag is primarily determined by the quality_bitmask. If the bitmask is non-zero or if any of the released data products have been filled then quality_flag=1. The bits in the bitmask are:

Bit 1. Set when accumulation is substantially shorter time than targeted. This data release accumulates 20 HIS normal mode scans (10 minutes) however due to interruptions from burst mode or spacecraft operations, accumulations can be shorter than this target.

Bit 2. Set when PAS proton solar wind speed is unavailable or highly varying. To limit the impact of time-of-flight accidentals, a velocity filter is used on the data. V02 uses a threshold equal to 70% the average PAS solar wind speed in the spacecraft frame during the HIS time accumulation.

Bit 3. Set when SSD filtering is unavailable or inaccurate. For a small fraction of individual elevation steps, HIS energy detector subsystem measurements may not be accurate. These instances are identified, removed, and corrected for when the high-resolution SSD sensor rate is available. However, during July and most of August 2022 only the low-resolution SSD sensor rate is available. Additionally, the identification of these

instances is less accurate when the instrument experiences strong temperature gradients.

Individual data products of a given record have a _qf=1 if either the uncertainty is large (signal-to-noise ratio < 1) and/or the record-level quality_flag=1. The HIS instrument team should be consulted before scientific publication with record-level quality_flag=1 data as the listed effects can influence the interpretation of these data.

In this version, time records are filled (quality_flag=2) if the number of accumulated scans <5 or filled manually after inspection at the discretion of the team. Individual released data products are filled separately. For O6+ bulk and thermal speeds, filled data indicates times when proton avoidance triggered too close to the O6+ VDF peak to calculate accurate moments via numerical integration. Filled data is expressed in the released data as a value of -1, as specified in the DPDD. Filled data may be available or made science-ready using non-standard or custom processing; contact the HIS instrument team about individual records or products.

2.7 Pre-2022 data

Prior to January 2022, noise levels in the HIS energy detector subsystem were high enough to produce significant artifacts in the data much of the time. These artifacts interfere with the accurate assignment of specific ions counts as well impact the quality filtering of the data using our current automated algorithms. Much of this data may be useful for scientific studies, however it requires substantially more manual validation. For this reason, it is not included in the current released data products.

Researchers investigating events prior to 2022 should contact the HIS team. It may be possible to provide composition data for specific short periods after manual validation and quality filtering.

3 Change Log

	16-Dec-2024	RMD, JMR, STL, HIS team	Initial V02 document version.