

National Aeronautics and Space Administration Goddard Earth Science Data Information and Services Center (GES DISC)

README Document for OMPS_NPP_NMHCHO_L2 and OMPS_N20_NMHCHO_L2

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1.0 Introduction

This document provides information for using Version 1.0 of the OMPS formaldehyde (HCHO) products derived from the Ozone Mapping and Profiler Suite Nadir Mapper (OMPS-NM) Level 1B spectra. The OMPS-NM HCHO products consist of orbital swath total vertical column densities of formaldehyde. The vertical columns are accompanied by support data consisting of uncertainty estimates, geolocation, quality flags and statistics, vertically resolved scattering weights, a priori formaldehyde profiles and ancillary data. This document aims to provide a basic summary and guide for using the data products. For detailed information on the algorithm, please see the Algorithm Theoretical Basis Document (ATBD).

1.1 Dataset and Instrument Description

1.1.1 OMPS Instrument Description

OMPS was launched on the Suomi National Polar-orbiting Partnership (SNPP) satellite on 28 October 2011, and on the JPSS-1 satellite (now known as NOAA-20) on 18 November 2017. OMPS/SNPP consists of the full OMPS suite of three instruments: 1) the OMPS nadir mapper (OMPS-NM), 2) the OMPS profile mapper (OMPS-NP) and 3) the OMPS limb profiler (OMPS-LP). OMPS/NOAA-20 consists only of the nadir package (OMPS-NM and OMPS-NP). The HCHO products described in this document are derived from Level 1B geolocated and calibrated radiance spectra from the OMPS-NM instruments.

The OMPS-NM instruments are hyperspectral nadir viewing spectrometers measuring backscattered light with a spectral resolution of ~1 nm (FWHM). OMPS/SNPP has a spectral range of 300 – 380 nm while OMPS/NOAA-20 measures from 300 – 420 nm. The instruments use 2-D CCD array detectors in pushbroom geometry to observe the two-dimensional field below the satellite's orbit over a swath width of ~2800 km. A detailed description of the instrument and the on-orbit performance of OMPS/SNPP can be found Flynn et al. (2014), Pan et al. (2017), and Seftor et al. (2014).

With 14 or 15 orbits per day, OMPS-NM provides daily global coverage of trace gas columns in the early afternoon local time, with NOAA-20's orbit behind that of SNPP by 50 minutes. Both satellites have a local equatorial crossing time of approximately 13:30. At nadir, OMPS/SNPP observations have a spatial resolution of 50 km \times 50 km, with a coarser resolution at the edges of the swath. Most OMPS/NOAA-20 observations have a nadir spatial resolution of 17 km \times 17 km up to 13 February 2019. On that date (orbit number 6419), the nominal spatial resolution was changed to 12 km \times 17 km. Some high-resolution observations were also collected during the early months of the OMPS/NOAA-20 mission.

1.1.2 OMPS NMHCHO dataset

OMPS HCHO consists of two products: 1) HCHO from OMPS on Suomi NPP (OMPS_NPP_NMHCHO_L2) and 2) HCHO from OMPS on NOAA-20 (OMPS_N20_NMHCHO_L2). OMPS/SNPP Level 2 HCHO data are available from January 2012 onwards, while OMPS/NOAA-20 data begin in January 2018. These products are processed with the same algorithm and nearly identical ancillary inputs. Each product contains the total vertical column density (VCD) HCHO, VCD uncertainty and quality flags, as well as support data used in the VCD derivation. The files also contain vertically-resolved scattering weights which describe the vertical sensitivity of the retrieval to different layers in the atmosphere.

1.1.3 Algorithm Background

The OMPS HCHO retrieval uses a three-step approach. First, we retrieve a differential slant column density, Δ SCD, of a trace gas in a nadir spectrum as compared to a clean reference spectrum using the OMPS L1B spectra (Jaross, 2017b). This is done by fitting a modeled spectrum to match the measured radiance spectrum of backscattered light in each ground pixel observation. For HCHO, we use a clean nadir reference spectrum determined from measurements over the Pacific. In the second step, we calculate an air mass factor (AMF) which describes the path of light through the atmosphere. The AMF is primarily a function of viewing geometry, aerosol and molecular scattering, surface reflectance, trace gas profile shape, cloud fraction and height, and of the strong absorption features of ozone in the UV which inhibit the penetration of photons close to the surface. Third, the retrieved SCD is corrected by adding the estimated background column SCD_{Ref} (determined from a chemical transport model) in the "clean" reference and for any remaining small latitude-dependent biases, SCD_B. These biases can sometimes occur at high latitudes due to unresolved calibration and spectroscopic issues. The final VCD is determined using:

$$VCD = \frac{\Delta SCD + SCD_{Ref} + SCD_B}{AMF}.$$

(1)

The AMF is calculated for each individual ground pixel using the VLIDORT radiative transfer model (Spurr, 2006) and climatological trace gas profiles from a 2018 GEOS-Chem global chemical transport model simulation at $0.5^{\circ} \times 0.5^{\circ}$ resolution at the time of overpass. The surface reflectance for the AMF uses an observation-geometry dependent bidirectional reflectance distribution function (BRDF) from MODIS (Schaaf et al., 2002; Wang et al., 2018), extended to the UV with surface albedo EOFs (Zoogman et al., 2016) and a SCIAMACHY surface albedo database (Tilstra et al., 2017). The surface reflectance over water is approximated using a Cox-Munk slope distribution.

While an independent cloud fraction and pressure retrieval is publicly available for OMPS/SNPP (Vasilkov et al., 2014), such a product does not currently exist for OMPS/NOAA-20. In order to be consistent between OMPS/SNPP and OMPS/NOAA-20 HCHO, the AMF calculation uses a cloud fraction derived from the OMPS-NM total ozone product reflectivity (Jaross, 2017a). The cloud pressure is from the total ozone product, which provides a cloud pressure climatology determined from OMI.

1.2 Data Disclaimer

Formaldehyde retrievals are provided for orbits that have valid publicly-available Level 1B calibrated radiances and total ozone files. As of June 2022, OMPS/SNPP L1B radiances and total

ozone were available through the GES DISC and OMPS/NOAA-20 radiances and total ozone were available through the OMPS website (<u>https://ozoneaq.gsfc.nasa.gov/data/omps</u>).

The OMPS instrument collects spectra on the dark side of the Earth for calibration purposes with a typical frequency of once per week. These orbit files will be twice as large in size as the nominal files. While the sunlit part of the orbit will contain valid data, the dark side of the orbit does not contain useful data. These ground pixels can be discarded using the main quality flag or a solar zenith angle (SZA) filter < 90°.

1.3.1 Data Citation and Acknowledgement

When using these data in your publication please cite the data product:

Gonzalo González Abad (2022), OMPS-NPP L2 NM Formaldehyde (HCHO) Total Column swath orbital, Greenbelt, MD, USA, Goddard Earth Sciences Data and Information Services Center (GES DISC), Accessed:[Data Access Date], 10.5067/IIM1GHT07QA8

Gonzalo González Abad (2022), OMPS-N20 L2 NM Formaldehyde (HCHO) Total Column swath orbital, Greenbelt, MD, USA, Goddard Earth Sciences Data and Information Services Center (GES DISC), Accessed:[Data Access Date], 10.5067/CIYXT9A4I2F4

References to the OMPS HCHO retrieval paper (Nowlan et al., 2022, in preparation) and the OMPS HCHO validation paper (Kwon et al., 2022, in preparation) should also be included in your publication.

1.3.2 Contact Information

Data inquiries should be addressed via email to Dr. Caroline Nowlan (cnowlan@cfa.harvard.edu) or Dr. Gonzalo González Abad (ggonzale@cfa.harvard.edu).

1.3 Quality Issues

Some orbits may be missing due to missing radiance files, missing total ozone files, satellite maneuvers or outages, invalid reference spectra, or other reasons. On occasion, Level 2 files may be available but do not contain valid data (usually appearing as NaN values) due to one of the above reasons or because of invalid geolocation or other input data.

2.0 Data Organization

Each OMPS HCHO file contains Level 2 swath data for a single orbit. There are typically 14 to 15 orbits per day.

Most OMPS/SNPP files have 36 pixels across the track and 400 pixels along the track.

Most OMPS/NOAA-20 files have either 104 pixels across the track and 1201 pixels along the track (prior to orbit 6419 on 13 February 2019), or 140 pixels across the track and 1201 pixels along the track (orbit 6419 and later).

2.1 File Naming Convention

OMPS HCHO files are named following the schema: <Sensor>-<Platform>_<Product>-<Level>_<Version>_<BeginDateTime>o<OrbitNumber>_<ProductionDateTime>.<suffix>

```
Where:

<Sensor> = OMPS

<Platform> = NPP or N20

<Product> = NMHCHO

<Level> = L2

<Version> = version number, e.g., v1.0

<BeginDateTime> = the start date and time in format <YYYYmMMDDtHHMMSS>

<OrbitNumber> = 6-character string representing orbit number (e.g., 005961)

<ProductionDateTime> = date and time of data production in format <YYYYmMMDDtHHMMSS>

<suffix> = nc
```

Filename example: OMPS-N20_NMHCHO-L2_v1.0_2019m0112t111052-o005961_2022m0517t211821.nc

2.2 File Format and Structure

The OMPS_NPP_NMHCHO_L2 and OMPS_N20_NMHCHO_L2 files are in netCDF (version 4) format. NetCDF is a set of software libraries and self-describing, machine-independent data formats that support the creation, access and sharing of array-oriented datasets. It was developed by UCAR/Unidata (<u>http://doi.org/10.5065/D6H70CW6</u>) https://www.unidata.ucar.edu/software/netcdf/.

The information is divided into five main groups:

- 1. key_science_data: the HCHO column, uncertainty and main data quality flag
- 2. **geolocation**: information on observation time, latitude, longitude, viewing and solar angles, time and terrain height at observation surface location
- 3. qa_statistics: fit convergence statistics and flags, RMS fitting residuals
- 4. **support_data**: support data used in the VCD calculation, including fitted slant column, air mass factor, cloud and surface information. This group also contains the vertically-resolved scattering weights.
- 5. uncertainty_budget: uncertainty estimates in key parameters

Orbital metadata are included as global keyword:value pairs.

Each orbital swath contains HCHO observations on a two-dimensional swath of ground pixels. These ground locations have dimensions *along_track* and *cross_track*. Fields with a vertical dimension additionally have a dimension *vertical_layer*. Fields that describe the latitude and longitude bounds of each ground pixel have the additional dimension *corner*. The dimension *vertical_level* is also given in the file. This defines the layer edges, where *vertical_level=vertical_layer+1*.

2.3 Key Science Data Fields

The variables included in the key_science_data group are the ones most likely to be used by users. These include the column_amount, column_amount_uncertainty and main_data_quality_flag. Other key data includes the scattering_weights in the support_data group. These can be used to recalculate AMFs with user-supplied profiles (Palmer et al., 2001) through:

$$AMF = \int_{z} w(z)S(z)dz$$
⁽²⁾

where w(z) is the scattering weight at layer z (provided in the file) and S(z) is the shape factor of the a priori profile, which is the partial column of HCHO in the layer normalized by the total column of HCHO (a new a priori profile can also be provided by the user).

Profile pressures can be reconstructed using the surface_pressure and its attributes eta_a and eta_b. The bottom boundary (pressure level) of a layer *i* is defined by:

$$p(i) = eta_a(i) + surface_pressure * eta_b(i)$$
(3)

with the top pressure level of the layer defined as:

$$p(i+1) = eta_a(i+1) + surface_pressure * eta_b(i+1).$$
(4)

Other key data fields for reconstruction of the column_amount (VCD) in Equation 1 include the support_group fields amf (AMF), fitted_slant_column_amount (Δ SCD), ref_sector_correction (SCD_{Ref}) and bias_correction (SCD_B).

3.1 Global Metadata

In addition to arrays containing geophysical quantities, support variables, and dimension scales, global metadata are also stored in the file. Some metadata are required by standard conventions, some are included to meet data provenance requirements and others as a convenience to users of the OMPS_NPP_NMHCHO_L2 and OMPS_N20_NMHCHO_L2 products. A summary of metadata global attributes present in all files is shown in Table 1.

| Global Attribute | Description | Туре |
|----------------------------------|--|--------|
| InputOriginalFile | Comma-separated list of input files used to generate the | string |
| | HCHO product (1, Level 1B radiance file, 2, Level 1B | |
| | radiance reference file, 3. Level 1B irradiance file – this is | |
| | not used for HCHO, 4. source of cloud information) | |
| ContactPersonEmail | Email address of the responsible person | string |
| ContactPersonName | Name of the responsible person | string |
| ContactPersonRole | Role of responsible person | string |
| contributor_name | Names of contributors | string |
| contributor_role | Roles of contributors | string |
| creator_email | Email of person principally responsible for creating this | string |
| | data | |
| creator_name | Name of person principally responsible for creating this | string |
| | data | |
| creator_role | Role of person principally responsible for creating this data | string |
| Conventions | CF metadata convention | string |
| DataSetQuality | Description of the data quality | string |
| Format | Format of data (netCDF-4) | string |
| id | Dataset identifier (same as ShortName) | string |
| IndentifierProductDOI | Product DOI identifier | string |
| IdentifierProductionDOIAuthority | http://dx.doi.org/ | string |
| institution | Name of institution responsible for originating data | string |
| instrument | Name of contributing instrument | string |
| instrument_vocabulary | Controlled vocabulary for names in "instrument" attribute | string |
| keywords | Comma-separated list of key words and phrases describing | string |
| | dataset | |
| keywords_vocabulary | Controlled vocabulary for names/phrases in "keywords" | string |
| | attribute | |
| LongName | Descriptive OMHCHO product name | string |
| metadata_link | URL to complete metadata | string |
| ObservationArea | Spatial coverage of the OMHCHO dataset | string |
| platform | Name of platform supporting sensor | string |
| platform_vocabulary | Controlled vocabulary for name in "platform" attribute | string |
| processing_level | Level of data processing | string |
| ProductGenerationAlgorithm | Algorithm software used to generate the file | string |

| ProductGenerationAlgorithmVersion | Version of the OMHCHO algorithm | string |
|-----------------------------------|--|----------|
| program | Overarching program of which dataset is a part | string |
| project | Comma-separated list of projects responsible for | string |
| | originating data | |
| references | References describing data and production | string |
| ShortName | Abbreviated name of the product | string |
| source | Instrument origin of the product | string |
| summary | Summary of dataset | string |
| title | Short phrase describing dataset | string |
| VersionID | ECS collection identifier | 32-bit |
| | | integer |
| license | License restriction ("Freely Distributed") | string |
| publisher_name | Name of group responsible for publishing data file | string |
| publisher_email | Email of group responsible for publishing data file | string |
| publisher_type | Type of publisher responsible for data file | string |
| publisher_url | Name of group responsible for publishing data file | string |
| publisher_institution | Institution responsible for publishing data file | string |
| OrbitNumber | Orbit number | 32-bit |
| | | integer |
| DayofYear | Day of year | 32-bit |
| | | integer |
| time_coverage_start | Time of first data point in dataset (format YYYY-MM- | string |
| | DDThh:mm:ss.sssZ) | |
| time_coverage_end | Time of last data point in dataset (format YYYY-MM- | string |
| | DDThh:mm:ss.sssZ) | |
| RangeBeginningDate | Date of first data point in dataset (format YYYY-MM-DD) | string |
| RangeBeginningTime | UTC time of first data point in dataset (format | string |
| | hh:mm:ss.sss2) | + |
| RangeEndingDate | Date of last data point in dataset (format YYYY-MM-DD) | string |
| RangeEndingTime | UTC time of last data point in dataset (format | string |
| | | <u> </u> |
| EquatorCrossingDate | Date of equator crossing time (format YYYY-MIM-DD) | string |
| EquatorCrossingTime | UIC time of equator crossing time (format nn:mm:ss.sss) | string |
| EquatorCrossingLongitude | Equator crossing longitude (degrees_east) | 32-DIt |
| | | noating |
| CranulalD | ONADE LICITO product filonomo | point |
| BroductionDateTime | Date and time of production (format VVVV MM | string |
| ProductionDaternine | DDThh:mm:ss sss7) | String |
| geospatial bounds | Polygons describing data's 2D geosnatial extent | string |
| | Coordinates are latitude (degrees north) and longitude | Jung |
| | (degrees east). | |
| history | Character array with line for each invocation of program | string |
| | that modified dataset | B |
| | | |

Table 1. File metadata

3.2 Variable Data Attributes

Table 2 shows a list of common data field metadata stored as attributes (keyword:values) for each variable. Not all metadata fields apply to all data fields. Table 3 gives attributes that only apply to specific data fields.

| Data Field Attribute | Description | Туре |
|----------------------|--|------------------|
| _FillValue | Fill value or missing value | data field type |
| long_name | Data field long name | string |
| comment | Additional description about the data field | string |
| units | Data field units (geophysical units or "1" for fraction) | string |
| valid_min | Data field minimum value. Values below valid_min should likely be discarded. | data field type |
| valid_max | Data field maximum value. Values above valid_max should likely be discarded. | data field type |
| coordinates | Dimension coordinates of the data field | string |
| _ChunkSizes | netCDF4 chunking size | unsigned integer |

Table 2. Common data field attributes

| Data Field Attribute | Data Fields Using Attribute | Description | Туре |
|----------------------------|--|---|-----------------------------|
| standard_name | geolocation/latitude geolocation/longitude geolocation/time | Standard name for data field | string |
| bounds | geolocation/latitude geolocation/longitude | Bounds of data field | string |
| flag_values | key_science_data/main_data_quality_flag qa_statistics/fit_convergence_flag | Possible flag values | data field type |
| flag_masks | support_data/glint_flag | Possible mask values | data field type |
| flag_meanings | key_science_data/main_data_quality_flag qa_statistics/fit_convergence_flag support_data/glint_flag | Definition of flag values | string |
| wavelength | support_data/amf | Wavelength at which AMF was calculated | 64-bit floating point |
| wavelength_unit | support_data/amf | Unit of wavelength attribute | string |
| radiance_reference_granule | support_data/ref_sector_correction | Level 2 file used in radiance reference correction | string |
| bias_granule | support_data/bias_correction | List of Level 2 files used in bias correction | string |
| eta_a | support_data/surface_pressure | Eta level A at pressure layer edge, with dimensions vertical_level | 64-bit floating point |

| eta_b | support_data/surface_pressure | Eta level B at | 64-bit |
|-------|-------------------------------|----------------------|----------|
| | | pressure layer edge, | floating |
| | | with dimensions | point |
| | | vertical_level | |

Table 3. Specific data field attributes

3.3 Dimensions

Table 4 lists dimensions associated with the data fields. Not all data fields use all dimensions. Only nominal dimensions are given (in particular, the along_track dimension varies occasionally).

| Global Attribute | Description | Nominal Dimensions |
|------------------|--------------------------------------|--------------------------------------|
| along_track | Number of ground pixels along the | 400 (NPP) |
| | satellite track | 1201 (NOAA-20) |
| cross_track | Number of ground pixels across the | 36 (NPP) |
| | satellite track | 104 (NOAA-20, Orbits 1 – 6418) |
| | | 140 (NOAA-20, Orbits 6419 – present) |
| corner | Number of corners in latitude and | 4 |
| | longitude bounds | |
| vertical_layer | Number of layers in data fields with | 47 |
| | vertical information | |
| vertical_level | Number of levels in data fields with | 48 |
| | vertical information | |

Table 4. Global file dimensions

4.0 Product

4.1 Data Fields

The following tables list the data fields in each group.

| Data Field Name | Description | Туре | Dimensions | Units |
|--------------------|--|------------------------------|-----------------------------|---------------------------|
| column_amount | HCHO column amount | 64-bit floating- point | along_track, cross_track | molecules/cm ² |
| column_uncertainty | HCHO column amount uncertainty. This is derived from the random uncertainty in the slant column spectral fit. | 64-bit floating- point | along_track, cross_track | molecules/cm ² |

4.1.1 key science data

| main_data_quality_flag | main data quality flag | 16-bit | along_track, | none |
|------------------------|------------------------|---------|--------------|------|
| | | integer | cross_track | |

Table 5: Data fields in key_science_data group

4.1.2 geolocation

| Data Field Name | Description | Туре | Dimensions | Units |
|------------------------|---|------------------------------|--|------------------|
| latitude | Latitude at pixel center | 32-bit floating- point | along_track, cross_track | degrees north |
| latitude_bounds | Latitude at pixel corners (SW,SE,NE,NW) | 32-bit floating- point | along_track, cross_track, corner | degrees north |
| longitude | Longitude at pixel center | 32-bit floating- point | along_track, cross_track | degrees east |
| longitude_bounds | Longitude at pixel corners (SW,SE,NE,NW) | 32-bit floating- point | along_track, cross_track, corner | degrees east |
| solar_zenith_angle | Solar zenith angle at pixel center | 32-bit floating- point | along_track, cross_track | degrees |
| solar_azimuth_angle | Solar azimuth angle at pixel center | 32-bit floating- point | along_track, cross_track | degrees |
| relative_azimuth_angle | Relative azimuth angle at pixel center | 32-bit floating- point | along_track, cross_track | degrees |
| terrain_height | Terrain height | 16-bit integer | along_track, cross_track | m |
| time | Exposure start time in seconds since 1993-01-01T00:00:00Z | 64-bit floating- point | along_track | seconds |
| viewing_zenith_angle | Viewing zenith angle at pixel center | 32-bit floating- point | along_track, cross_track | degrees |
| viewing_azimuth_angle | Viewing azimuth angle at pixel center | 32-bit floating- point | along_track, cross_track | degrees |

Table 6: Data fields in geolocation group

4.1.3 qa_statistics

| · | | | | |
|----------------------|--------------------------------------|------------------------------|-----------------------------|-------|
| Data Field Name | Description | Туре | Dimensions | Units |
| fit_convergence_flag | Slant column fit convergence flag | 16-bit integer | along_track, cross_track | none |
| fit_rms_residual | Normalized radiance fit RMS residual | 64-bit floating- point | along_track, cross_track | none |

| num_good_input | Number of pixels for which | 32-bit | 1 | none |
|------------------------|------------------------------|-----------|---|------|
| | slant column fitting is | integer | | |
| | attempted | | | |
| percent_bad_output | Percent of num_good_input | 32-bit | 1 | % |
| | flagged as "bad" in main | floating- | | |
| | quality flag | point | | |
| percent_good_output | Percent of num_good_input | 32-bit | 1 | % |
| | flagged as "good" in main | floating- | | |
| | quality flag | point | | |
| percent_suspect_output | Percent of num_good_input | 32-bit | 1 | % |
| | flagged as "suspect" in main | floating- | | |
| | quality flag | point | | |

Table 7: Data fields in *qa_statistics* group

4.1.4 support_data

| Data Field Name | Description | Туре | Dimensions | Units |
|---------------------------------|-------------------------------|-----------|--------------|---------------------------|
| albedo | Geometry-dependent | 32-bit | along_track, | none |
| | surface Lambertian- | floating- | cross_track | |
| | Equivalent Reflectivity. This | point | | |
| | is not used in the AMF | | | |
| | calculation but is given to | | | |
| | help user estimate effective | | | |
| | surface reflectivity. | | | |
| amf | Calculated air mass factor | 32-bit | along_track, | none |
| | | floating- | cross_track | |
| | | point | | |
| bias_correction | Bias correction | 32-bit | along_track, | molecules/cm ² |
| | | floating- | cross_track | |
| | | point | | |
| brdf_geo | Amplitude of Li-Sparse | 32-bit | along_track, | none |
| | BRDF kernel | floating- | cross_track | |
| | | point | | |
| brdf_iso | Amplitude of isotropic BRDF | 32-bit | along_track, | none |
| | kernel | floating- | cross_track | |
| | | point | | |
| brdf_vol | Amplitude of Ross-Thick | 32-bit | along_track, | none |
| | BRDF kernel | floating- | cross_track | |
| | | point | | |
| cloud_fraction | Effective cloud fraction used | 32-bit | along_track, | none |
| | in AMF computation | floating- | cross_track | |
| | | point | | |
| cloud_pressure | Cloud pressure used in AMF | 32-bit | along_track, | hPa |
| | computation | floating- | cross_track | |
| | | point | | |
| fitted_slant_column_amount | Fitted slant column density | 64-bit | along_track, | molecules/cm ² |
| | | floating- | cross_track | |
| | | point | | |
| fitted_slant_column_uncertainty | Fitted slant column density | 64-bit | along_track, | molecules/cm ² |
| | uncertainty | floating- | cross_track | |
| | | point | | |

| gas_profile | A priori gas mixing ratio profile used in AMF calculation | 32-bit floating- point | vertical_layer, along_track, cross track | none |
|-----------------------|---|------------------------------|--|---------------------------|
| glint_flag | Flag for possible glint | byte | along_track, cross_track | none |
| ice_fraction | Sea ice fraction | 32-bit floating- point | along_track, cross_track | none |
| land_fraction | Land fraction | 32-bit floating- point | along_track, cross_track | none |
| meridional_wind | Meridional wind | 32-bit floating- point | along_track, cross_track | m/s |
| ocean_salinity | Ocean salinity in Practical Salinity Units (PSU) | 32-bit floating- point | along_track, cross_track | g/kg (1e-3) |
| ref_sector_correction | Reference sector background correction | 32-bit floating- point | along_track, cross_track | molecules/cm ² |
| scattering_weights | Scattering weights | 32-bit floating- point | vertical_layer, along_track, cross track | none |
| snow_fraction | Snow fraction | 32-bit floating- point | along_track, cross_track | none |
| surface_pressure | Surface pressure | 32-bit floating- point | along_track, cross_track | hPa |
| temperature_profile | Temperature profile | 32-bit floating- point | vertical_layer, along_track, cross_track | К |
| zonal_wind | Zonal wind | 32-bit floating- point | along_track, cross_track | m/s |

Table 8: Data fields in *support_data* group

4.1.5 uncertainty_budget

| Data Field Name | Description | Туре | Dimensions | Units |
|------------------------|--|------------------------------|-----------------------------|---------------------------|
| amf_total_uncert | Total AMF uncertainty. This field is empty in Version 1. | 32-bit floating- point | along_track, cross_track | % |
| bias_uncertainty | Estimated uncertainty in bias correction, assuming AMF uncertainty of 50% | 32-bit floating- point | along_track, cross_track | molecules/cm ² |
| ref_sector_uncertainty | Estimated uncertainty in reference background correction, assuming AMF uncertainty of 50% | 32-bit floating- point | along_track, cross_track | molecules/cm ² |

Table 9: Data fields in uncertainty_budget group

4.2 Quality Control

Most users should filter data by key_science_data/main_data_quality_flag. Pixels flagged as "bad" are almost certainly not useful. Pixels flagged as "suspect" may still be usable in some cases but should be used with caution.

<u>Pixels are flagged as "suspect" if any of the following criteria are met:</u> snow_fraction > 0 ice_fraction > 0 column_amount + 2*column_amount_uncertainty < 0 AMF_G > 4

```
Pixels are flagged as "bad" if any of the following criteria are met:

|column_amount| > 2e17 molecules/cm<sup>2</sup>

column_amount + 3*column_amount_uncertainty < 0

amf < 0.1

AMF<sub>G</sub> > 5
```

Where the geometric air mass factor is: AMF_G = sec(solar_zenith_angle) + sec(viewing_zenith_angle)

We recommend that most users further limit the use of HCHO data to SZA < 70° and cloud fractions < 0.4. At large SZA, the signal-to-noise is severely degraded and low radiance spectra typically show more biases in the retrieval. At higher cloud fractions, the systematic uncertainties become very large. In addition, we recommend users filter out ground pixels over ice and snow using the ice and snow fractions in the support data. The ice and snow fractions are not currently used for the AMF calculation, but are included for convenience in data interpretation. While slant column retrievals over these surfaces are usually valid, the cloud fraction retrievals may be unable to differentiate between a bright surface and clouds and will therefore be inaccurate.

5.1 Command Line Utilities

ncdump

With ncdump it is possible to generate CDL text representations of OMPS HCHO netCDF datasets. A full description of the capabilities of ncdump can be found here: <u>https://www.unidata.ucar.edu/software/netcdf/netcdf/ncdump.html</u> To quickly explore the structure of an OMPS HCHO file, outputting it to struc.txt, issue the following command:

ncdump -c <filename> > struc.txt

or if coordinate variable values (longitude and latitude) are not desired in the ouput:

ncdump -h <filename> > struct.txt

5.2 Tools/Programming

HDFView

HDFView is a Java-based graphical user interface created by the HDF Group, which can be used to browse the OMPS HCHO files. The utility allows users to view all objects in an HDF file hierarchy, which is represented as a tree structure. HDFView documentation and downloads are available at <u>https://www.hdfgroup.org/downloads/hdfview/</u>

Panoply

OMPS HCHO datasets are geo-referenced and can be visualized using Panoply, a Java based graphical user interface capable of plotting arrays from netCDF files. Further information and download options are available at https://www.giss.paca.gov/tools/papoply/

https://www.giss.nasa.gov/tools/panoply/

netCDF programing interfaces are available for major high-level languages including IDL, Matlab, R, and Python.

6.0 GES DISC Data Services

OMPS HCHO products are archived and distributed by the Goddard Earth Science Data & Information Services Center (GES DISC). The files can be directly downloaded from the GES DISC or search using NASA's EarthData web services which provides capabilities for spatial and temporal subsetting. GES DISC provides a list of tools that can read netCDF-4 files. To download GES DISC data you must (1) register in Earthdata Login and (2) be authorized for NASA GES DISC Data Access.

Registering and downloading data with Earthdata can be achieved here: <u>https://disc.gsfc.nasa.gov/</u>

If you need assistance or wish to report a problem: **Email:** gsfc-dl-help-disc@mail.nasa.gov **Voice:** 301-614-5224 **Fax:** 301-614-5268 **Address:**

Goddard Earth Sciences Data and Information Services Center, NASA Goddard Space Flight Center Code 610.2 Greenbelt, MD 20771 USA

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| Acronym | Meaning |
|-----------|---|
| AMF | Air Mass Factor |
| ATBD | Algorithm Theoretical Basis Document |
| BRDF | Bidirectional reflectance distribution function |
| CDL | Common Data Language |
| CF | Climate and Forecast |
| DOI | Digital Object Identifier |
| ECS | EOSDIS Core System |
| EOF | Empirical Orthogonal Function |
| EOS | Earth Observing System |
| EOSDIS | EOS Data and Information System |
| FWHM | Full width at half maximum |
| GEOS-Chem | Goddard Earth Observing System chemical transport model |
| GES DISC | Goddard Earth Sciences Data and Information Services Center |
| HDF | Hierarchical Data Format |
| JPSS | Joint Polar Satellite System |
| L1B | Level-1B (calibrated radiances or irradiances) |
| L2 | Level-2 (retrieved geophysical values) |
| LP | Limb Profiler |
| MEaSUREs | Making Earth Science Data Records for Use in Research |
| | Environments |
| MODIS | Moderate Resolution Imaging Spectroradiometer |
| N20 | NOAA-20 |
| NE | Northeast |

Appendix A. List of Acronyms

| NetCDF | Network Common Data Form |
|-----------|--|
| NM | Nadir Mapper |
| NOAA | National Oceanic and Atmospheric Administration |
| NP | Nadir Profiler |
| NW | Northwest |
| OMI | Ozone Monitoring Instrument |
| OMPS | Ozone Mapping and Profiling Suite |
| RMS | Root Mean Square |
| SCD | Slant Column Density |
| SCIAMACHY | SCanning Imaging Absorption spectroMeter for Atmospheric |
| | CHartographY |
| SE | Southeast |
| SIPS | Science Investigator-led Processing System |
| SNPP | Suomi National Polar-orbit Partnership |
| SW | Southwest |
| SZA | Solar Zenith Angle |
| UCAR | University Corporation for Atmospheric Research |
| UTC | Universal Time Coordinated |
| VCD | Vertical Column Density |
| VLIDORT | vector linearized discrete ordinate radiative transfer |

Table 10. List of acronyms and abbreviations.