JEM/SMILES Level-2 Product Guide for v3.2 (118-12-0702)

Version 1.1

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JEM/SMILES L2 Products Guide

Table of Contents

PREFACE

The Superconducting Submillimeter-Wave Limb-Emission Sounder (SMILES) was developed for use aboard the Japanese Experiment Module (JEM) on the International Space Station (ISS) through the cooperation of the Japan Aerospace Exploration Agency (JAXA) and the National Institute of Information and Communications Technology (NICT). SMILES was successfully launched on an H-IIB rocket with an H-II Transfer Vehicle on 11 September, 2009, was attached to the JEM on 25 September, and began atmospheric observations on 12 October. Mission objectives are as follows: (1) to demonstrate a 4 K mechanical cooler and superconducting mixers in the environment of outer space for submillimeter limb-emission sounding in the frequency bands of 624.32–626.32 GHz and 649.12–650.32 GHz and (2) to globally measure minor atmospheric constituents in the middle atmosphere (O_3, HCl, ClO, HO_2, HOCl, BrO, O_3 isotopes, HNO_3, CH_3CN, etc.) to gain a better understanding of factors and processes controlling the amount of stratospheric ozone and the relationship with climate change. Unfortunately, SMILES observations had been suspended since 21 April 2010 owing to the failure of a critical component in the submillimeter local oscillator. Although the observation period was limited to about six months, SMILES had been performing global observations at about 100 locations per ISS orbit, except for some restrictions due to ISS operation. After data processing, we had global and vertical distributions of about 10 minor atmospheric constituents related to ozone chemistry. In this document we will demonstrate the capability of obtaining high-quality scientific data which will be important in addressing scientific issues such as the ozone depletion problem, middle atmosphere chemistry with a special focus on the diurnal cycle, and the transport process for minor species. We hope the output from SMILES will demonstrate its high potential to observe minor atmospheric constituents in the middle atmosphere.

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Principle Investigator of the SMILES mission team

1. PURPOSE OF THE DOCUMENT

Researchers and scientists in atmospheric sciences can use this document to understand the quality and characteristics of the data from Superconducting Submillimeter-wave Limb-emission Sounder (SMILES) on the basis of SMILES standard level 2 (L2) products processed and provided by JAXA.

This product guide provides the following:

1) Descriptions of SMILES observations.
2) Descriptions of the latest SMILES L2 products.
3) Descriptions of data format.

2. SMILES OBSERVATION AND DATA PROCESSING

2.1. INTRODUCTION TO SMILES

The Superconducting Submillimeter-wave Limb-Emission Sounder (SMILES) was launched on September 11, 2009 as a joint project between the Japan Aerospace Exploration Agency (JAXA) and the National Institute of Information and Communications Technology (NICT), and was attached to the Japanese Experiment Module (JEM) on the International Space Station (ISS) on September 25, 2009. For details of SMILES configurations, see the SMILES Mission Plan, version 2.1, at http://darts.isas.jaxa.jp/iss/smiles/docs/SMILES_MP_ver2-1.pdf. SMILES carries 4 K cooled Superconductor-Insulator-Super-conductor (SIS) mixers to carry out high-sensitivity measurements for submillimeter limb-emission sounding. Since the system noise temperature of SMILES is nearly 350 K, the sensitivity of SMILES is much higher than that of similar sensors in orbit. For general post-launch information, you may consult Kikuchi et al. (2010a, 2010b) and Ochiai et al. (2010); some important information on SMILES measurement is summarized in Table 2.2.

SMILES measures atmospheric limb emission from minor constituents within the submillimeter-wave region from 625 GHz to 650 GHz for three specified detection bands: 624.32–625.52 GHz (Band A), 625.12–626.32 GHz (Band B), and 649.12–650.32 GHz (Band C). Target species and sample spectra are shown in Table 2.1, Figure 2.1-, and Figure 2.1-. SMILES instruments only consist of two AOS spectrometers. Accordingly, observations of Bands A, B, and C are made on a time-sharing basis. Depending on the combination, the AOS spectrometer for Band A may be switched.

Table 2.1-1 Major characteristics of SMILES (*Ochiai et al.*, 2012).

System parameter	Description
Frequency bands	624.26 – 625.59 GHz (Band A) 625.06 – 626.38 GHz (Band B) 649.05 – 650.38 GHz (Band C)
Frequency resolution	1.05 - 1.20 MHz (FWHM)
Number of channels	1728 for each unit of AOS
Channel separation	approx. 0.8 MHz
Integration time	0.47 s for each observation point
Calibration period	53 s

System parameter	Description
System noise temperature	297 - 380 K
Temperature resolution	0.30 - 0.42 K (for line spectrum) 0.18 - 0.27 K (for continuum)
Beam width	0.089 deg. (V) x 0.173 deg. (H) (FWHM)

Table 2.1-2 SMILES target species in level-2 data processing.

Band	**Band A** (624.32–625.52GHz)	**Band B** (625.12–626.32GHz)	**Band C** (649.12–650.32GHz)
Target Species	O_3 HCl ($H^{37}Cl$) ^{18}OOO HNO_3 CH_3CN HOCl $O^{17}OO$ BrO	O_3 HCl ($H^{35}Cl$) ^{18}OOO $O^{17}OO$ HO_2	O_3 ClO HNO_3 ^{18}OOO ^{17}OOO HO_2 BrO

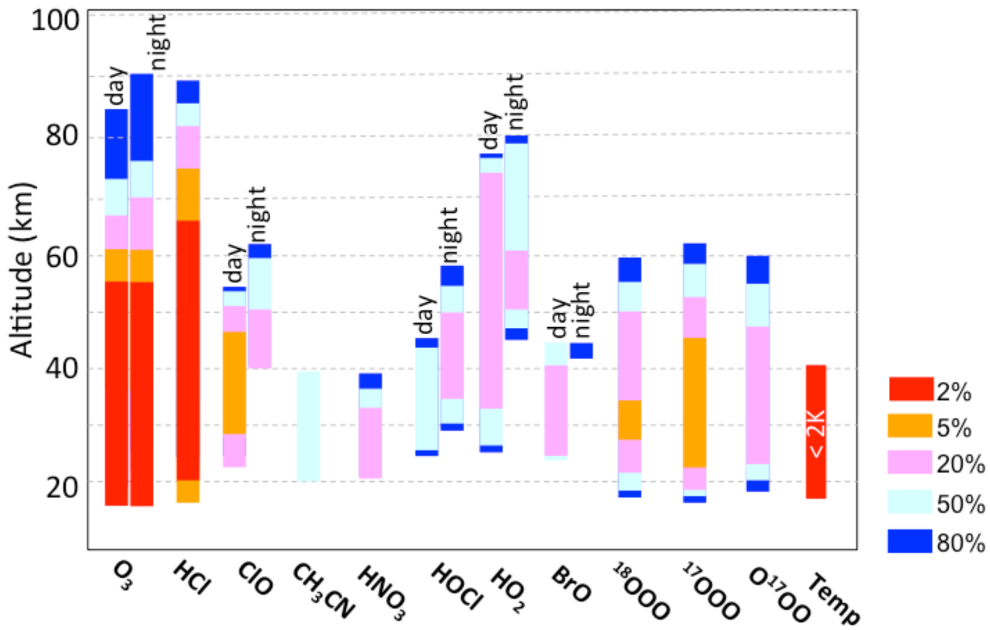

Figure 2.1-1 Theoretical precision ratios (single scan) by *a priori* profile (November 2009 and Northern middle-latitude case).

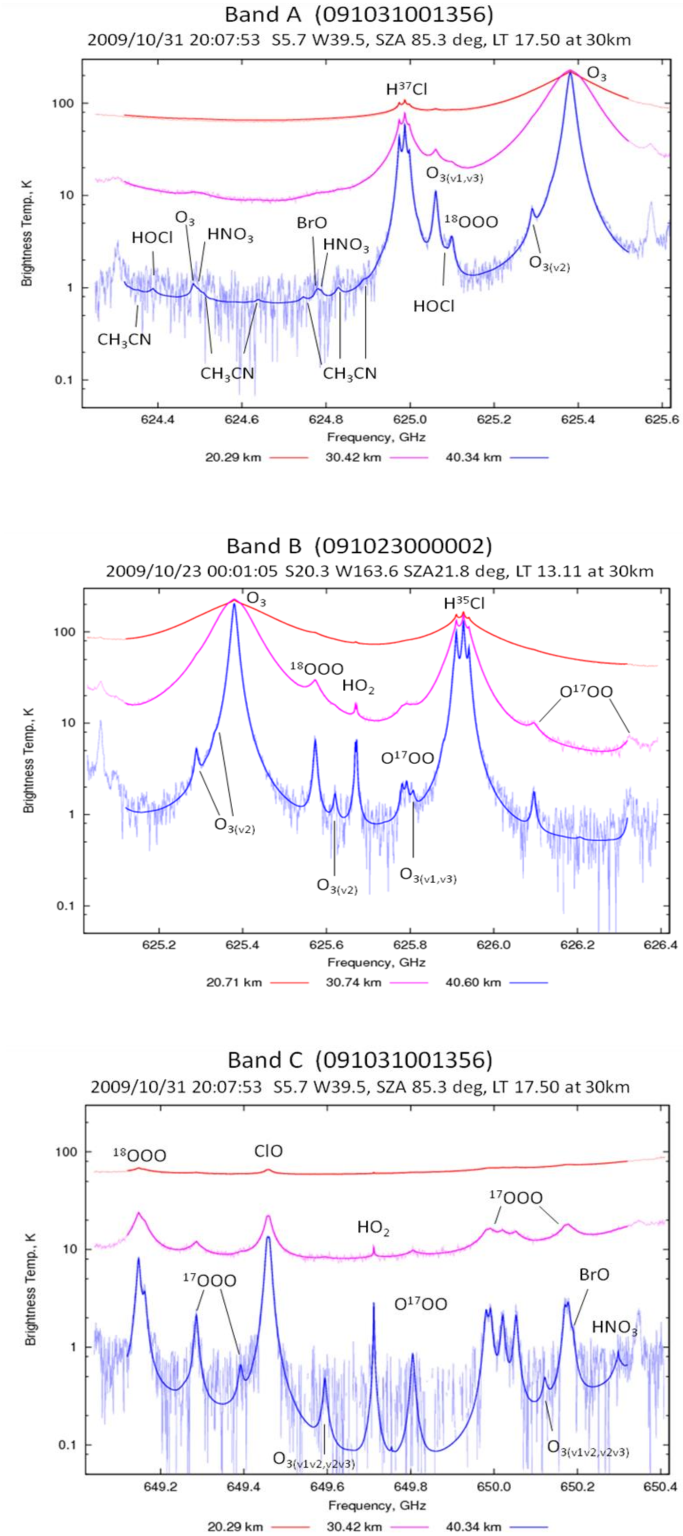

Figure 2.1-2: Samples of observed and fitted spectra (thin lines: observed, thick lines: fitted) in each band (*Suzuki et al., 2012*).

2.2. SMILES OBSERVATION

The ISS has a circular orbit with an inclination angle of 51.6°, and is located at an altitude of about 400 km above the Earth's surface. While it circles the Earth at 90 minutes per orbit, atmospheric observations are being conducted. The SMILES antenna is tilted 45° to the left from the direction of orbital motion. This design enables SMILES to observe latitudes from 38°S to 65°N.

Figure 2.2 shows an example of globally mapped ozone distribution at 28 km on 20 March, 2010. Original observation points are plotted using white circles with observed ozone mixing ratios. White circles without color indicate missing data points rejected as abnormal values. It was discovered that SMILES performed observations continuously, but we can see that there are specific latitudes where the data is missing. This is due to solar paddle interference that occurred twice in one circular orbit.

The observation period was from October 12, 2009 to April 21, 2010. The first few weeks until November 6 were used as a trial period before going into full SMILES operational mode. During this period, the ratio of missing data was quite high. In addition, the AOS thermal control heaters were turned off gradually therefore we need to be careful of differing characteristics in SMILES data in the trial compared with the following observation period. Details of data availability, its quality, and valid latitude range are summarized in Table 2.2 and Figure 2.2.

Another important aspect of SMILES observations is that SMILES can measure the atmosphere at different local times because of the non-sun-synchronous ISS orbit. ISS local time precession takes about two months to cover the whole day therefore we may calculate diurnal variations by combining the data from the ascending and descending nodes on the basis of a one month period approximately (Figure 2.2-1).

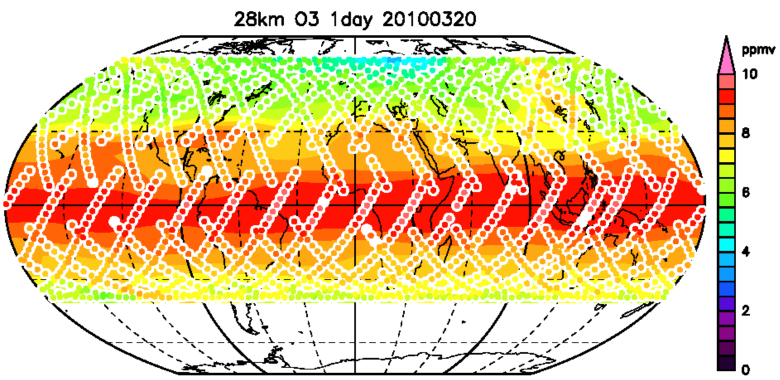

Figure 2.2-1 Measurement points for a day.

Table 2.2-1 Irregular data from SMILES L2 product.

Period	Event	Data number	Ratio of un-useable scans	Latitude coverage
2009/10/12 – 11/06	Trial period	almost normal	almost normal	normal
2009/10/12 – 23	AOS thermal control heaters turned on.	-	-	-
2009/10/24 – 26	Some AOS thermal control heaters turned on.	-	-	-
2009/10/27 –	AOS thermal control heaters turned off.	-	-	-
2009/11/19 – 11/24	ISS yaw maneuver (Atlantis docking)	normal	normal	opposite direction
2009/11/30 – 12/15	ISS solar paddles stopped just in front of SMILES IFOV	normal	high	normal
2010/02/10 09:00 - 2010/02/19 23:59	ISS yaw maneuver (Endeavour docking)	normal	normal	opposite direction
2010/02/24 00:00 - 2010/03/05 15:00	Trouble with ISS/JEM communication system	low (10% of normal level)	normal	normal
2010/04/07 11:00 - 2010/04/17 11:59	ISS yaw maneuver (Discovery docking)	normal	normal	opposite direction

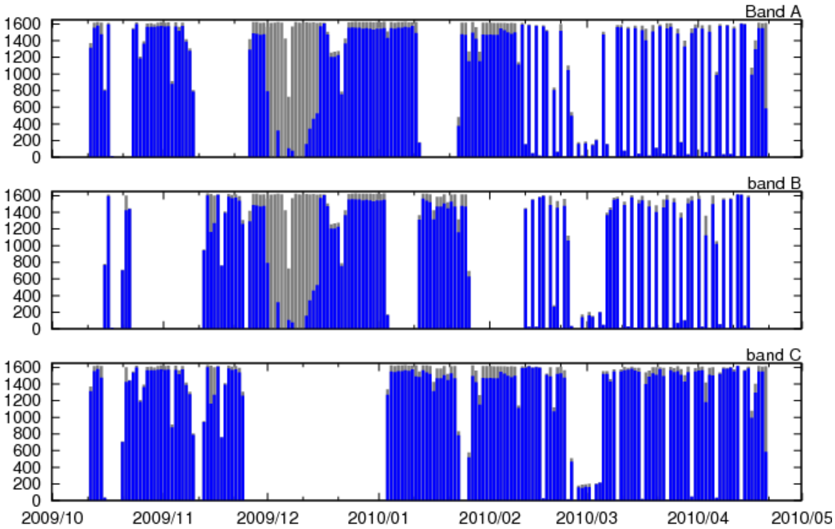

Figure 2.2-2 Observation numbers per day for Bands A, B, and C. Gray regions show total observations; blue regions show available numbers after discarding abnormal scans such as those due to field obstacles indicated by L1B information (L1B 008).

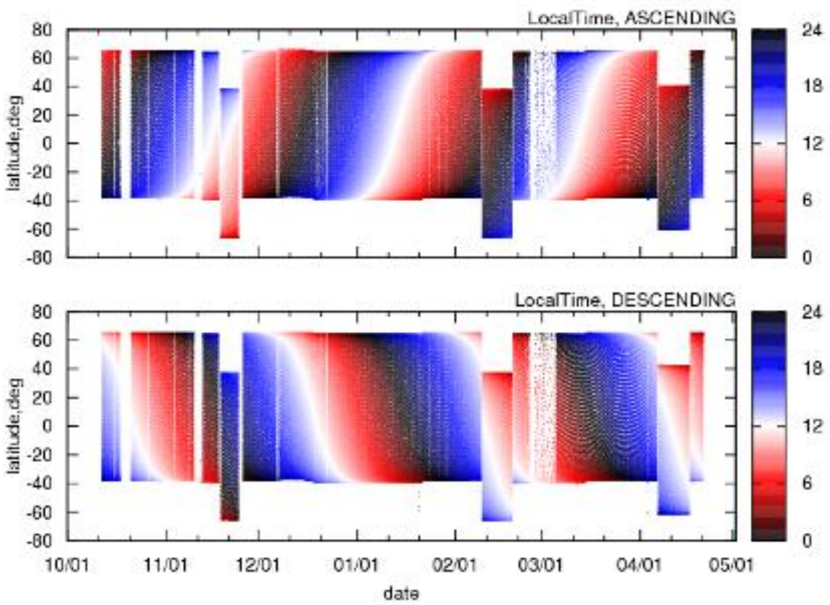

Figure 2.2-3 Latitude and time series of local time at SMILES observation points.

2.3. SMILES GROUND DATA SYSTEM

Data observed by SMILES is multiplexed with data from other JEM experiments. Multiplexed data is downlinked from the ISS through geostationary data relay satellites to ground receiving stations. SMILES data is processed from RAW data to L0 data at the User Operation Area at JAXA/TKSC. SMILES L0 data is provided to the DPS-L0/L1 Data Processing System for the SMILES Ground Data System.

L0 data is converted into calibrated limb spectral radiance using calibration data in the L0/L1 data processing system (DPS-L0/L1). Anomalous data is checked and flagged before processing. Ancillary data such as tangent altitude and position of the observation are created and added as a part of L1 data products. L1 data is transferred to the L2 Data processing system (DPS-L2) via the network and converted into L2 data which consists of concentration profiles of targeted gases, temperature and pressure. Standard L2 data processing is performed at JAXA/ISAS.

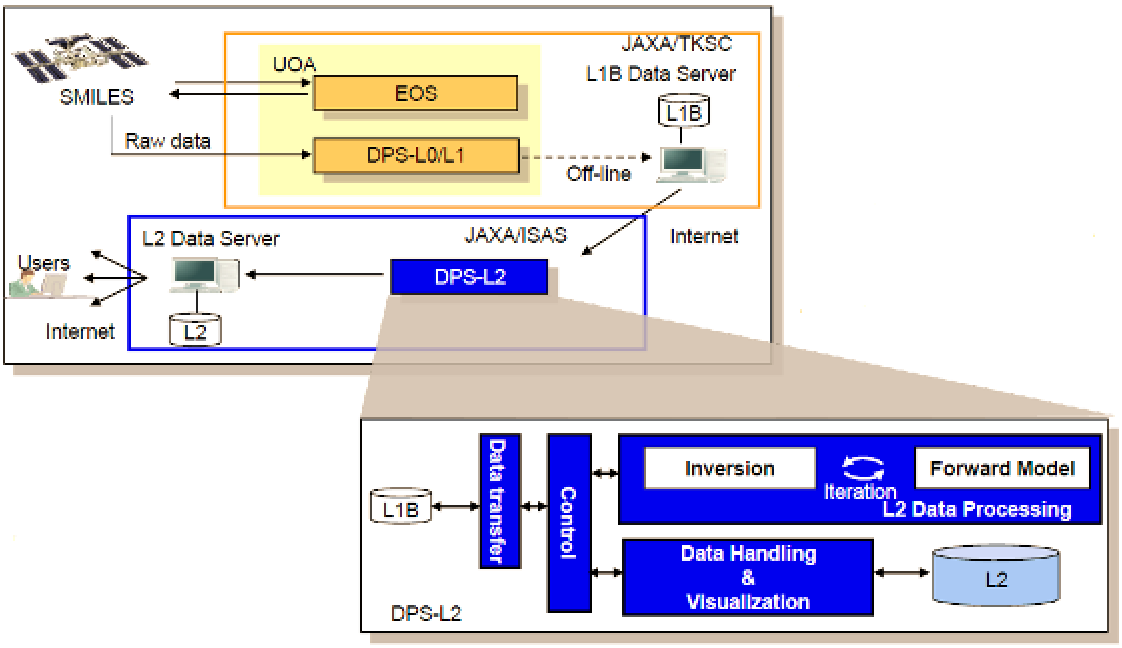

Figure 2.3-1 SMILES ground data system.

2.4. RETRIEVAL ALGORITHM

In this document we only describe brief information of the SMILES retrieval algorithm. It is based on the optimal estimation method followed by Rodgers (1976, 1990, 2000). The details of the retrieval algorithm for the DPS-L2 can be found in separate technical papers (Takahashi et al., 2010, 2011). In the v2.2 update of the SMILES L2 product, the Tikhonov regularization method level 1 (Doicu et al., 2010) has been implemented in combination with the optimal estimation method for the retrieval of O_3, HCl and HNO_3 (Manago et al., 2013). In the v3.0 update and later, a combined use of the optimal estimation method and the Tikhonov regularization method level 2 has been applied for the retrieval of all species. See Subsection 2.6 for brief product release history and more details in Appendix A.1

2.5. A PRIORI DATASET

For operational L2 processing, we prepared 7 sets of a priori data calculated from 5 data sources including satellite data, reanalysis data, and output from chemistry transport models (Table 2.5-1, Table 2.5-2).

Table 2.5-1 *A priori* datasets.

Data set	Description
Climatology	
Aura/MLS	Monthly average for 2005-2007 from EOS-Aura/MLS v2.2 [*Froidevaux et al.*, 2008]. Latitude bin is 10 degrees, and day-time and night-time sets were prepared separately for O_3,ClO, HOCl, HO_2, BrO.
UARS/MLS	Monthly average for 1992-1994 from UARS/MLS. Latitude bin is 10 degrees.
CCSR/NIES	Monthly average of CCMVal-REF2 output for 2001-2010 from CCSR/NIES CCM [*Akiyoshi et al.*, 2009, 2010]. Latitude bin is 10 degrees, and hourly sets in local time were prepared for O_3, ClO, HOCl, HO_2, BrO.
SD-WACCM	Monthly average for same month from SD-WACCM CCM [*Kunz et al., 2011*] nudged with GEOS-5. Latitude bin is 1.8 degrees, and hourly sets in local time were prepared for all parameters.
Nearest data	
GEOS-5	Reanalysis data produced by NASA/GMAO's GEOS-5 DAS [*Rienecker et al.*, 2008] included Aura/MLS O_3 and Temperature. The grid is 2.0 deg latitude x 2.5 deg longitude with 3-hour intervals; closest time and location data is used with 4-point spatial interpolation.
SD-WACCM	CCM Simulations from SD-WACCM nudged with GEOS-5 (not including Aura/MLS). The grid is 1.9 deg latitude x 1.25 deg longitude with 0.5-hour intervals; closest time and location data on the grid is used.
AURA/MLS	Gridded data for same day from Aura/MLS v2.2. Latitude-longitude grid is 5.0 x 5.0 degrees; closest location data is used with 4-point spatial interpolation.

Table 2.5-2 List of *a priori* dataset.

data	Climatology data				Nearest data		
	Aura /MLS	UARS /MLS	CCSR /NIES	SD-WACCM	GEOS-5	SD-WACCM	Aura /MLS
O_3	○		-	●		-	
HCl	○		-	●		-	
ClO	○		-	●		-	
HNO_3	○		-	●		-	
CH_3CN		-		●		○	
HOCl	-		○	●		-	
HO_2	-		○	●		-	
BrO	-		○	●		-	
Temp.	-		-	-	●○	-	●○
Pres.	-		-	-	●○	-	
Wind			-	-	●○	-	
H_2O	-		-	-	●○	-	

(-: existing data / ○: used data in v2.4 processing / ●: used data in v3.2 processing)

2.6. PRODUCT RELEASE HISTORY

We have updated our L2 product almost every six months in the first several years after the launch. The following descriptions are brief summaries for each version of the L2 products. See details in Appendix A.1.

Hereafter, in the 9 digit number in the description for each version “XXX-YY-ZZZZ”, “XXX” shows the L1B data version number, “YY” shows that of *a priori* datasets, and “ZZZZ” shows that of L2 retrieval algorithms.

- v1.0 (005-06-0024): for retrieval tests (released 23/01/2010)
  V1.0 is a test processing version in order to check L2 processing algorithms designed before launch [Takahashi et al., 2010].

- v1.1 (005-06-0032): for mapping tests (released 19/04/2010)
  Pointing data was improved to increase the amount of useful data and to create gridded data.
- v1.2 (005-06-0150): algorithm update I (released 15/09/2010)
  We included experimental correction factors in the AOS response function (one of the instrumental functions), resulting that retrieved temperature agrees with TIMED/SABER to suppress internal inconsistency between receivers.
- v1.3 (006-06-0200): algorithm update II (released 02/03/2011)
  This version is the first update in L1B processing algorithms (For details, see level 1 Product Release Notes (Ver.006)). Screening conditions during solar paddle interference are well defined, so abnormal values during such conditions can be properly selected.
- v2.0 (007-08-0300): major update (released 04/10/2011)
  The L1B version was updated to ver. 007 by introducing non-linearity correction. This reduced the bias of stratospheric temperature, resulting in an 8% decrease in O_3 at peak height level as well as other improvements in L2 products (Mitsuda et al., 2011).
- v2.1 (007-08-0310): improvements to HOCl (released 16/01/2012)
  This was a minor update to aim to improve HOCl by re-investigating line data around HOCl. We have released this version of the data to the public (05/03/2012).
- v2.2 (007-09-0400): algorithm update
  Retrieval height range was re-investigated in order to obtain proper results in the upper mesosphere and the lower thermosphere, and smoothing of the retrieved profiles was taken into account using the Tikhonov Regularization method (TRM).
- v2.3 (007-09-0402): status flag update
  Screening conditions were re-evaluated, and the useful data rate was improved by around 30-50 %.
- v2.4 (008-11-0502): a priori profile update (released 03/07/2013)
  Retrieval settings were modified to improve O_3 profiles in the lower thermosphere.
- v3.0 (118-12-0602): algorithm update and L1B data modification (released 15/11/2013)
  Bias data for some species were suppled. Modified L1B data (v118) were introduced and the inversion model was updated.
- v3.1 (118-12-0602): systematic update
  Missing data due to errors occurred in data processing were recovered.

- v3.2 (118-12-0702): algorithm update (released 10/04/2017)
  Smoothing parameters and a prior errors used in the inversion model were adjusted to suppress the oscillation of retrieved profiles.

3. LATEST UPDATES FOR SMILES L2 PRODUCTS

3.1. SUMMARY OF ALGORITHM UPDATES

In the recent product (v3.2), the following points have been improved in comparison with v2.4 product. In Section 3.3 information about the averaging kernels of v2.4 and v3.2 is provided. In Appendix A.1 you may see details about the updates of earlier versions.

- Bias data for ClO, BrO and HO_2: Night-time bias data for ClO, BrO, HO_2 are included as ancillary data. See the Product Guide (v2.4) for details of retrieval method of the bias.

- Calibrated brightness temperature (Level 1B processing): L1B product has some problems about the correction of non-linearity in brightness temperature calibration. In second-latest L2 product (v2.4) the latest L1B product (v008) was used, but we found that differences of O_3 and HCl profiles between the AOSs increased, especially in the data observed in October, 2009. Therefore we produced another L1B product (v118) in which brightness temperature is same as second-latest L1B product (v007). The v3.0 and later versions were produced based on L1B v118 product.

- Improvement of inversion model: In v2.4, O_3, HCl, HNO_3 had been retrieved with the combination of Optimal Estimation method (OEM) and Tikhonov Regularization method (TRM) Level 1, while other species had been retrieved with only OEM. For the v3.2 product, combination of OEM and TRM level 2 is applied for retrieval of all species. In addition, because of HNO_3 (band C) profiles with oscillations affecting BrO profiles larger regularization factors are applied.

- The followings have been modified in the inversion model with introduction of the TRM:
  - Altitude grid for retrieval is set to 2.5km for all species.
  - Altitude correlation of OEM is set to 0.01km for all species.
  - Climatology data of SD-WACCM is used as a priori data for all parameters except meteorological values. (See Table 2.5-2)
  - The integral value of averaging kernel within +/- 5km of target altitude grid has been adopted as the criterion for determining of "useful altitude range",

with whose threshold set to 0.6. Users can screen the useful altitude range with the criteria “***L2Precision*** < 0”, which is not changed from the previous products.

- Modification in the product format: ***InformationValueLimited*** is newly added to the product HDF field, which means the integral value of averaging kernel around +/- 5 km of target altitude grid. (See Table 4.4-2)。

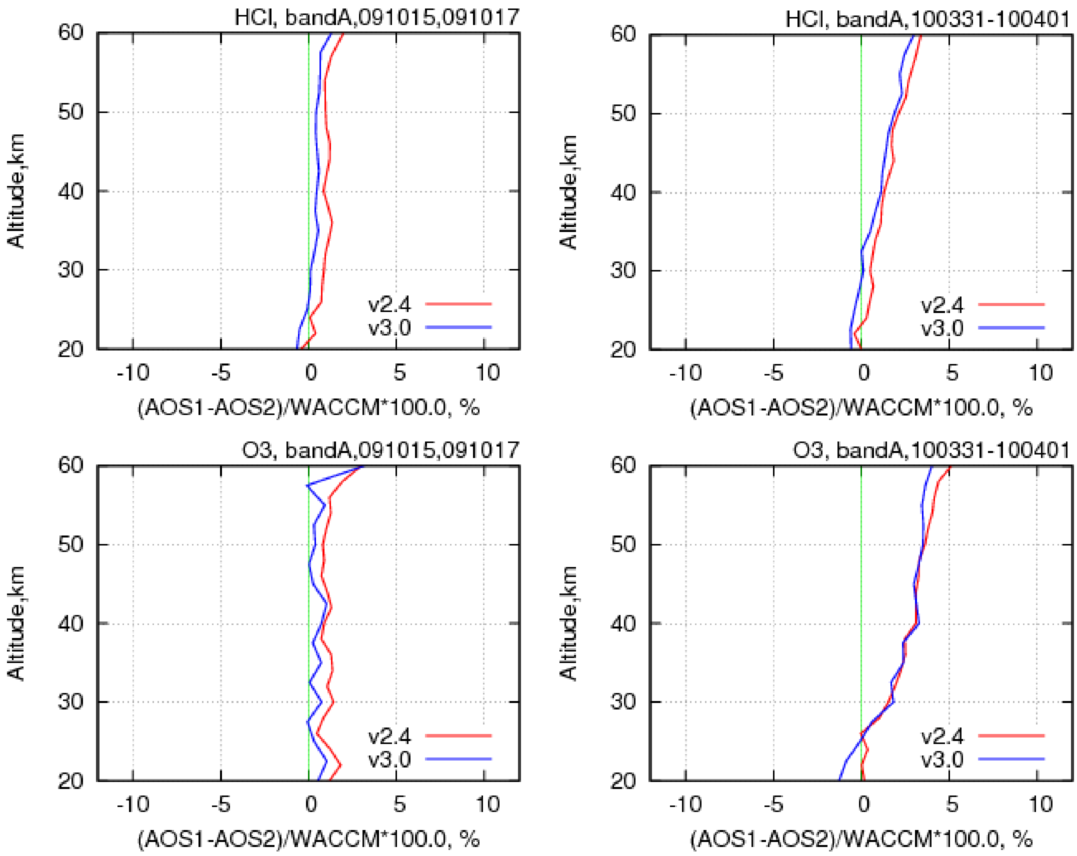

Figure 3.1-1 Relative difference between HCl profiles in L2 v2.4 and v3.0. (left: 2009/10/15 and 10/17, right: 2010/03/31 and 04/01. The upper panels for HCl, and the lower for O3. See Imai et al., (2013) for the calculation method of the difference.

3.2. USEFUL DATA

The amounts and ratios of useful data for v3.2 are shown in Table 3.2-1.

Table 3.2-1 Useful data for v3.2

	Number			Ratio (%)		
	A	B	C	A	B	C
v3.2	136003	99253	144658	85.49	78.21	81.47

3.3. Profile differences between v3.2 and v2.4

3.3.1 O_3

SMILES observes ozone by detecting strong absorption lines at 625.37GHz with Bands A and B, and the wings of absorption lines at 647.8GHz and 650.8GHz with Band C. Band C is suitable for measuring ozone near the tropopause because there are few strong lines in the band. Since only spectrum data above 15 km are considered in the present version of the retrieval process, Band C has few advantages. The signal-to-noise ratio of ozone lines detected with Bands A and B is highest among any absorption lines measured by the SMILES spectroscopy system; theoretical random error is lower than 1% at the altitude of 20 – 50 km.

The validation of O_3 data in the v2.1 product was done by comparison with satellite-borne data, CTMs (SD-WACCM and MIROC3.2-CTM) and ozonesonde data (Imai et al., 2013a, 2013b). It was found that this data agrees within 10% difference in the stratosphere and 30% difference in the mesosphere. In addition, the diurnal components of O_3 agree well with the results of SD-WACCM and MIROC3.2-CTM. These results have been used in the analysis of diurnal variation of stratospheric and mesospheric ozone (*Sakazaki et al.*, 2013).

Figure 3.3-1 and Figure 3.3-2 show the difference between v2.4 and v3.2 for sample profiles and averaging kernels.

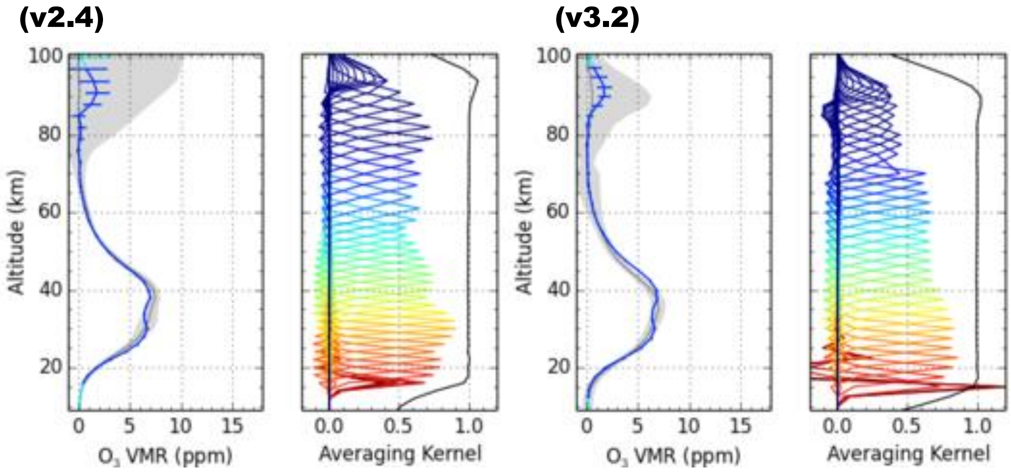

Figure 3.3-1 Sample profiles and averaging kernels for O_3 (daytime, band A). Left: An aqua line shows a retrieved profile in all altitude and a blue line shows a retrieved profile in useful range. Error bars show theoretical retrieval precisions. A gray line shows a priori profile and shaded region shows range of *a priori* error. Right: Colored lines show the averaging kernel and a black line shows integrated averaging kernel.

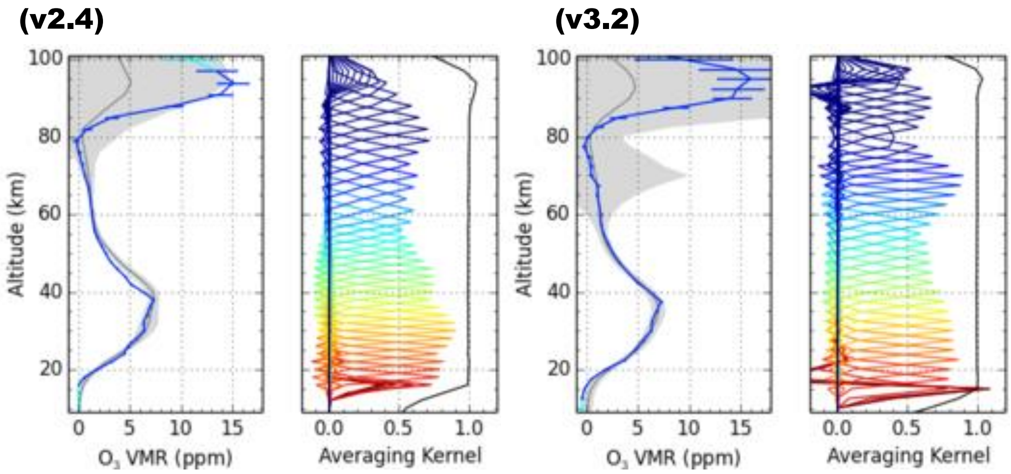

Figure 3.3-2 O_3 (nighttime, band A) as in Figure 3.3-1.

3.3.2 HCL

For HCl, SMILES detected $H^{37}Cl$ with Band A and $H^{35}Cl$ with Band B. Since the absorption line in Band B is stronger than that of Band A, retrieval results from Band B have better sensitivity at higher altitudes.

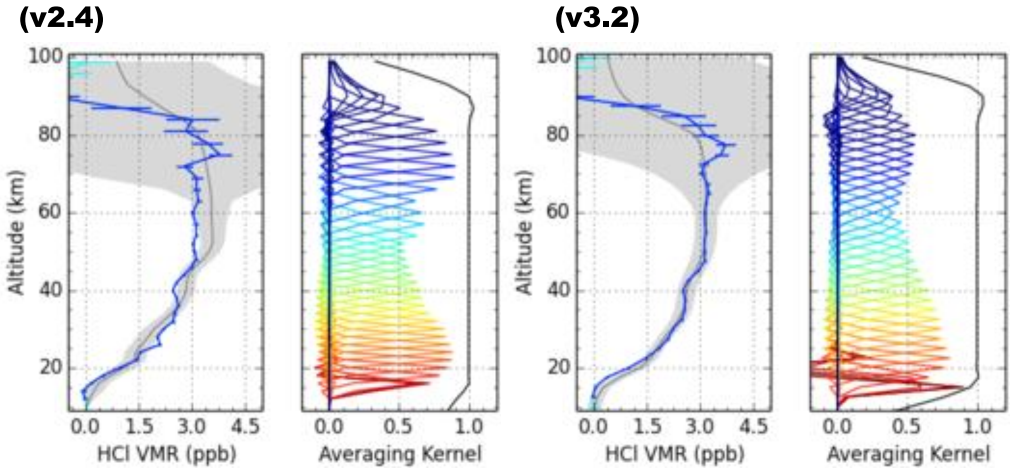

Figure 3.3-3 HCl (band B) as in Figure 3.3-1.

3.3.3 ClO

As ClO can be detected with highest sensitivity in Band C, the differences in single profiles between daytime and night-time can be distinguished (see Figure 3.3-4). Suzuki et al. (2012) reported that ClO v1.2 agrees with Aura/MLS v2.2 in the stratosphere. ClO v1.3 profiles had been compared with ground-based millimeter-wave spectrometer data, and it was reported that the agreement was good at altitudes of up to 40 km (Kuwahara et al., 2012).

Figure 3.3-5 shows the averaging kernels of v2.4 data for daytime, and Figure 3.3-6 for night-time. According to these results, the profiles are “usable” at altitudes up to 70 km for both daytime and night-time, and sensitivity is high in that altitude range.

In the lower altitude region (<35 km), the SMILES ClO product shows night-time bias. ClO values should be zero below 35 km, but it shows a bias due to instrumental effects (Suzuki et al., 2012). This bias can be corrected by subtracting night-time zonal mean value, as already demonstrated in the case of BrO (Stachnik et al., 2013). Since the bias values change seasonally and with latitude, it is recommended that correction should be done in monthly basis with a 10° latitude bin. These may be related to the fact that SMILES Acousto-Optic Spectrometer characteristics were changed after October 23, 2009 when laser diode temperature levels changed.

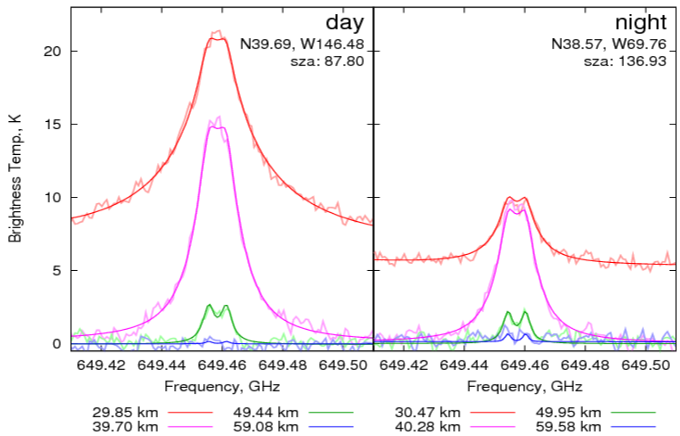

Figure 3.3-4 Examples of ClO spectra (November 2009 and mid-latitude). Thick lines show L2 spectra and thin lines show L1B (observed) spectra.

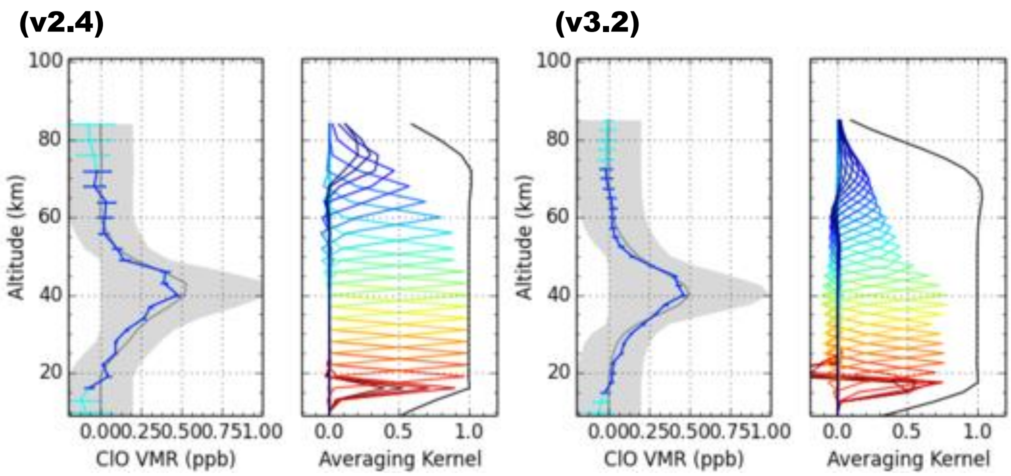

Figure 3.3-5 ClO (daytime, band C) as in Figure 3.3-1.

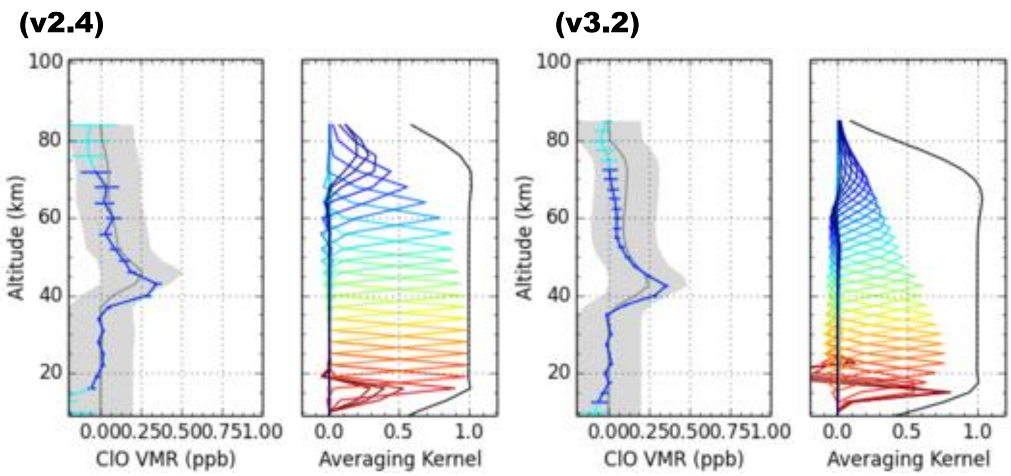

Figure 3.3-6 ClO (nighttime, band C) as in Figure 3.3-1.

3.3.4 HNO_3

HNO_3 can be detected with Bands A and C, but there is calibration error due to the line being positioned at the observation band in Band C, and there is some errors due to the spectral wing of HCl in Band A.

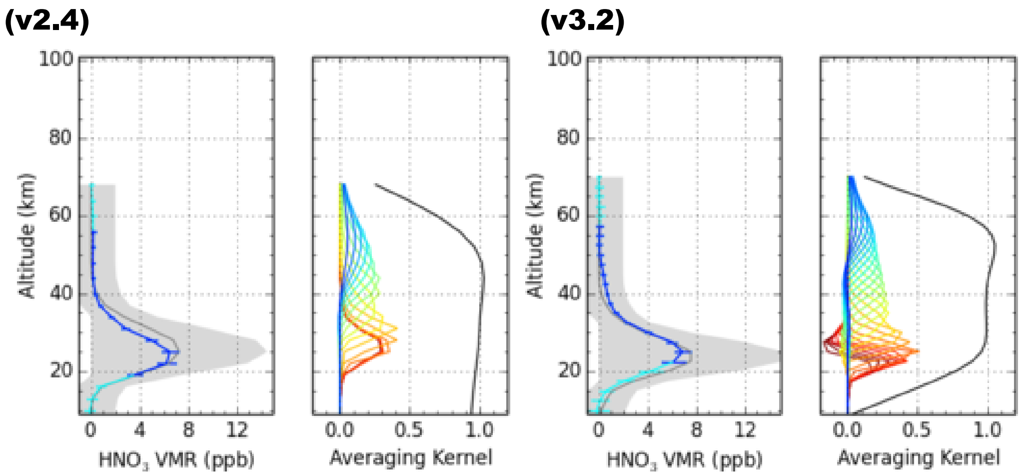

Figure 3.3-7 HNO_3 (band C) as in Figure 3.3-1.

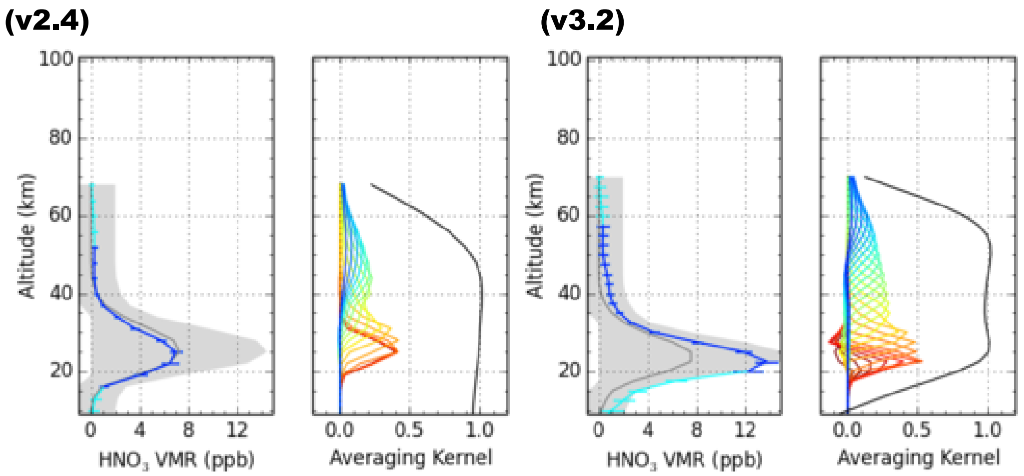

Figure 3.3-8 HNO_3 (band A) as in Figure 3.3-1.

3.3.5 HOCL

HOCl can be detected with Band A, but its spectral line is positioned at the shoulder of excited O_3 and O_3 isotopes (See Figure 3.3-9). Therefore HOCl retrieval is affected by O_3 line parameter and calibration errors in the lower stratosphere. In the v3.2 retrieval process, SD-WACCM climatological data is adopted as *a priori* profiles instead of CCSR/NIES climatological data.

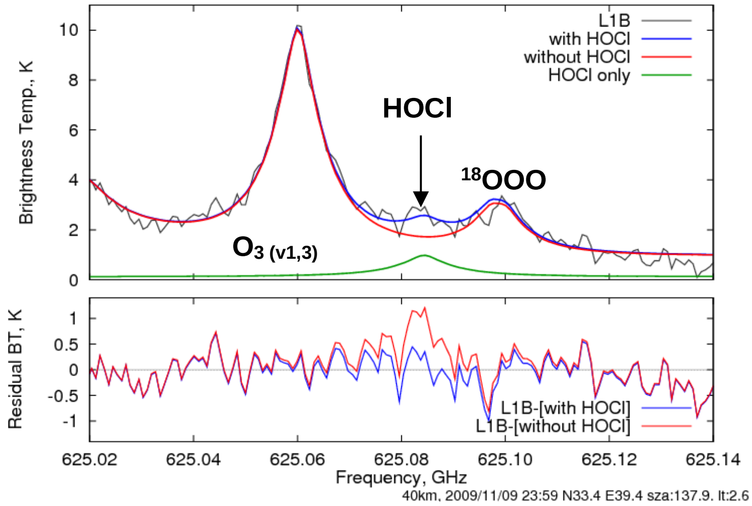

Figure 3.3-9 Example of HOCl Spectrum at 40km.

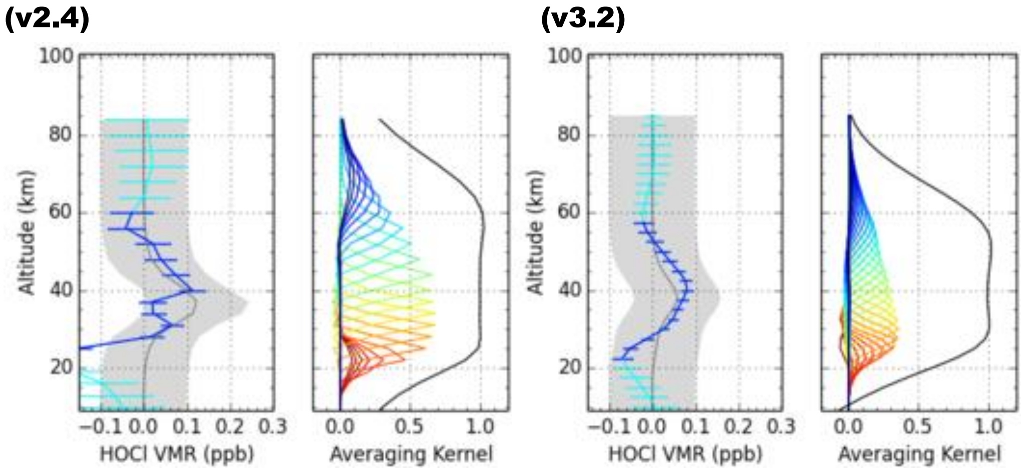

Figure 3.3-10 HOCl (daytime, band A) as in Figure 3.3-1.

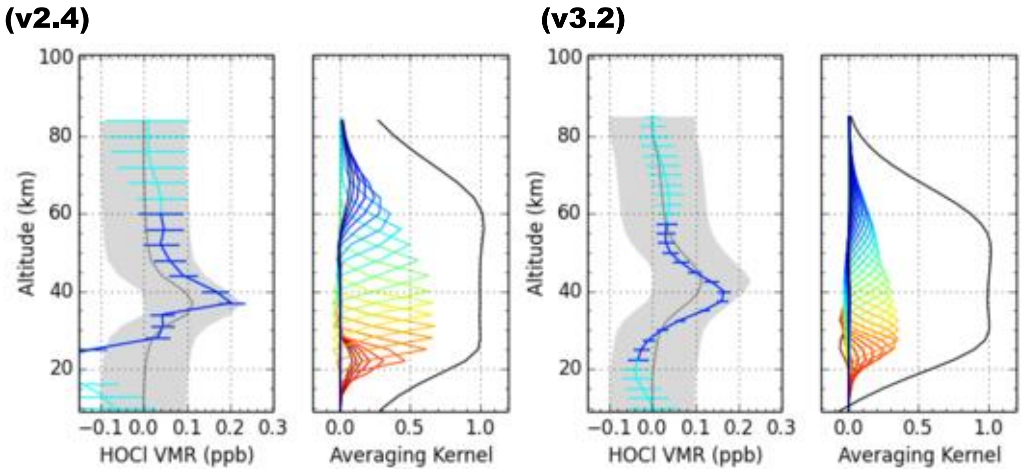

Figure 3.3-11 HOCl (nighttime, band A) as in Figure 3.3-1.

3.3.6 CH_3CN

CH_3CN can be detected only with Band A, but its retrieval is affected by the spectral wing of HCl lines. After v2.4 retrieval, only the nearest grid data of SD-WACCM calculations is adopted as an a priori value.

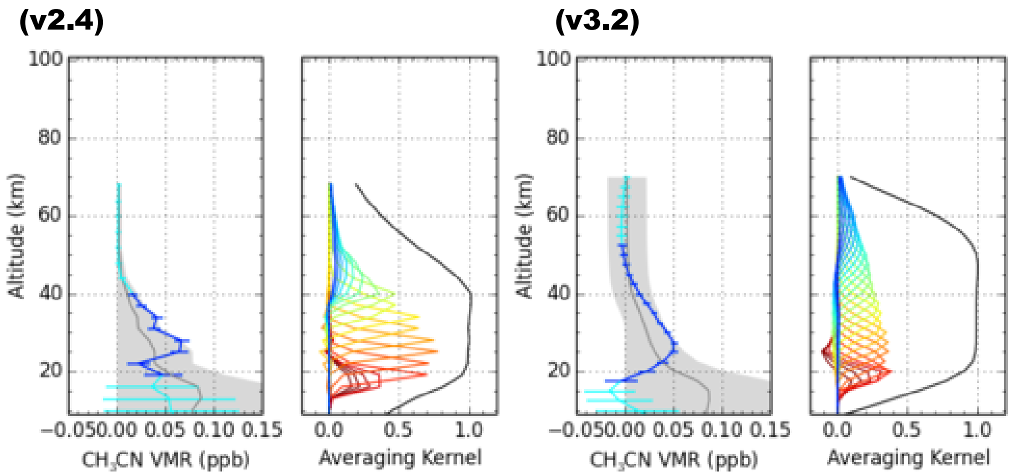

Figure 3.3-12 CH_3CN (band A) as in Figure 3.3-1.

3.3.7 BrO

BrO can be detected with Bands A and C. Among lines overlapping with the BrO line, the ozone isotope line in Band C is the most intense. As the ozone isotope is retrieved using other lines of different frequencies (See Figure 3.3-13), it is recommended that BrO results from Band C are used.

Similar to the case of ClO, the BrO product shows night-time bias. This bias can be corrected by subtracting night-time zonal mean value, as already demonstrated by Stachnik et al. (2013). Since the bias values change seasonally and with latitude, it is recommended that correction should be done in monthly basis with a 10° latitude bin. These may be related to the fact that SMILES Acousto-Optic Spectrometers' characteristics were changed after October 23, 2009 when laser diode temperature levels changed.

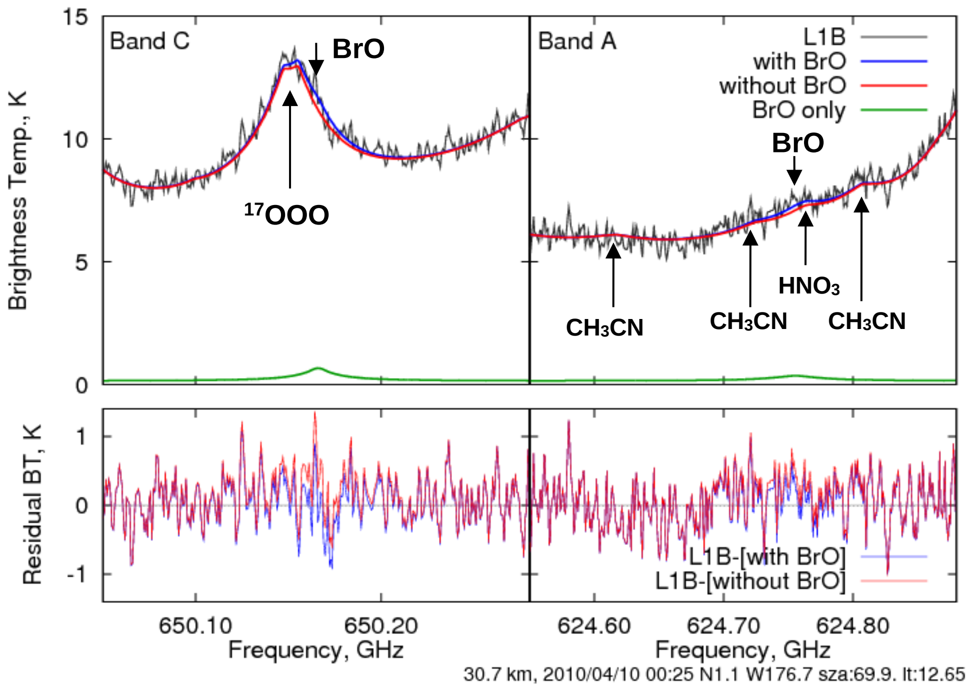

Figure 3.3-13 Examples of BrO spectrum at 30 km.

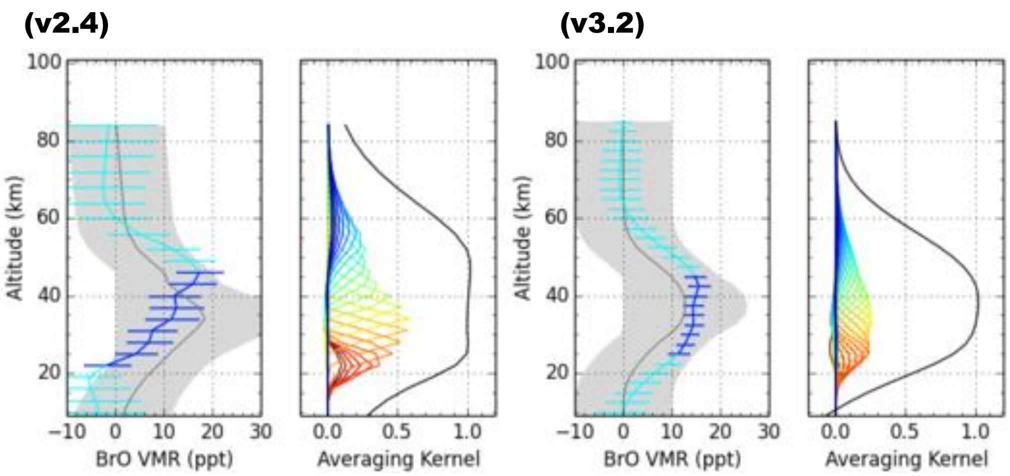

Figure 3.3-14 BrO (daytime, band C) as in Figure 3.3-1.

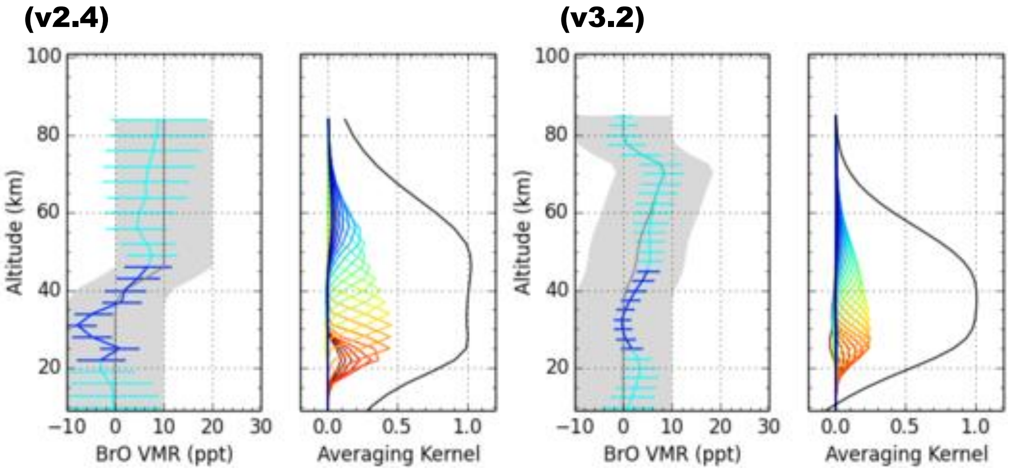

Figure 3.3-15 BrO (nighttime, band C) as in Figure 3.3-1.

3.3.8 HO_2

HO_2 can be detected with Bands B and C, and there are independent spectral lines with comparable intensity in both bands (See Figure 3.3-16). From v2.4 retrieval, a priori errors have been extended, so that HO_2 can be retrieved up to an altitude of 90 km. As a result, there was a peak of around 80 km in the profiles which had not been recognized with older versions of the product (see Figures 3.3-17 and 3.3-18). However, stratospheric values in HO_2 profiles still have different biases in each band and these will be re-evaluated in further studies in a similar manner to BrO profiles.

Similar to the cases of ClO and BrO, HO_2 value should be zero below 35 km at night-time. However, we see a bias due to instrumental effects (*Suzuki et al.*, 2012). This bias can be corrected by subtracting night-time zonal mean value, as already shown in the case of BrO (*Stachnik et al.*, 2013). Since the bias values change seasonally and with latitude, it is correction should be done in monthly basis with a 10° latitude bin.

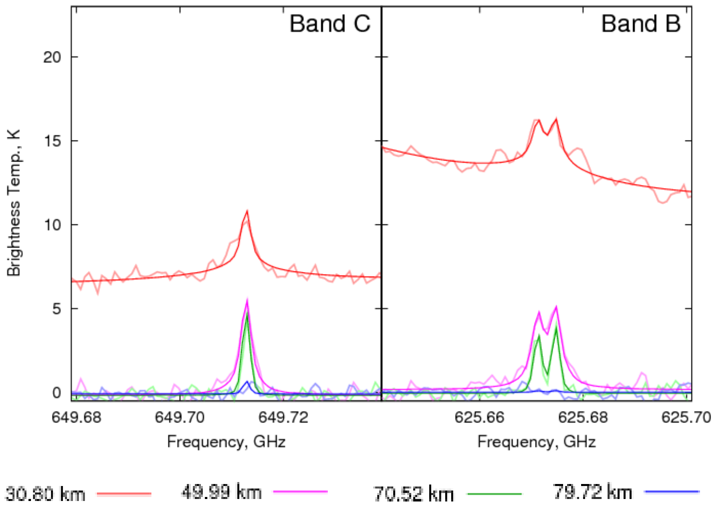

Figure 3.3-16 Examples of HO_2 Spectra (in November and near the Equator). Thick lines show L2 spectra and thin lines show L1B (observed) spectra. Left: Band C and right: Band B

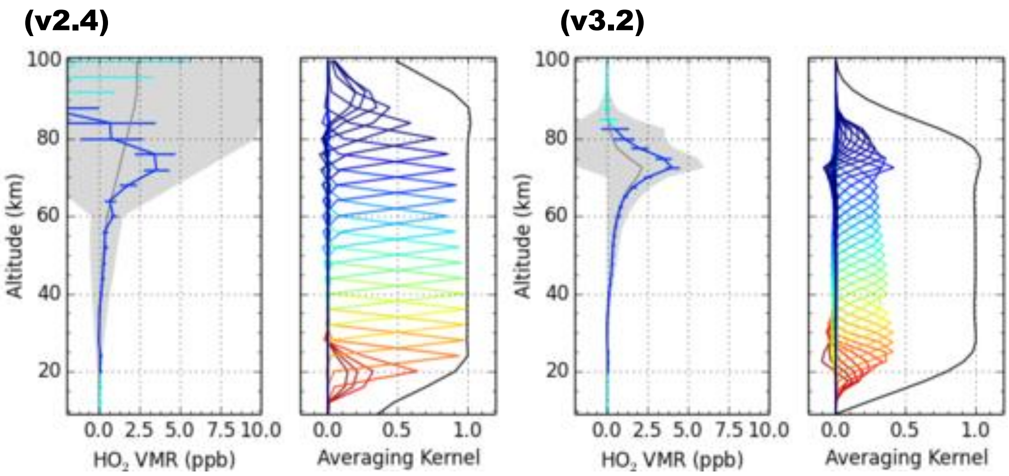

Figure 3.3-17 HO_2 (daytime, band B) as in as Figure 3.3-1.

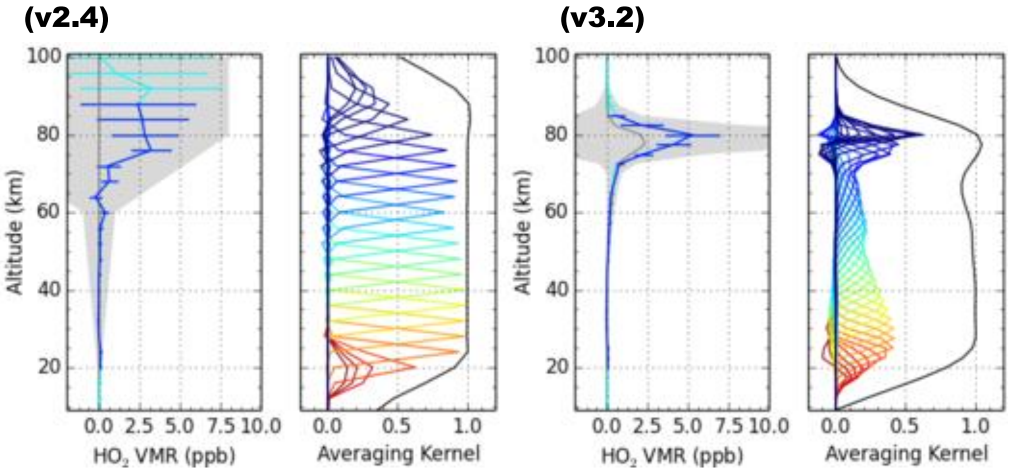

Figure 3.3-18 HO_2 (nighttime, band B) as in Figure 3.3-1.

3.3.9 TEMPERATURE

There is no measurable spectral line of O_2 in the SMILES observation bands, so temperature profiles are retrieved with O_3 and HCl lines in Bands A and B. After the v2.1 algorithm, *a priori* data with small errors has been directly referred in the retrieval process in order to avoid errors with retrieving mesospheric temperature. The v3.2 algorithm follows the principle adopted in v2.4 (GEOS-5 data which is nudged with Aura/MLS temperature and O_3 data up to the mesosphere has been adopted up to 60km, and tidal effects have been calculated within GEOS-5 data. For altitudes higher than 60km, the nearest grid in Aura/MLS climatology data is directly referred to as *a priori*).

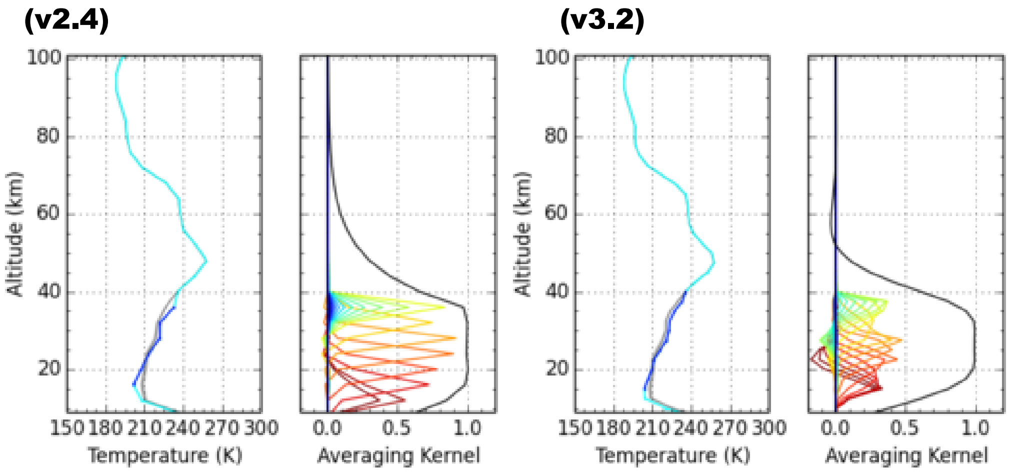

Figure 3.3-19 Temperature (band B) as in Figure 3.3-1.

3.3.10 O_3 ISOTOPES

SMILES can detect 3 out of 4 types of O_3 isotope excluding $O^{18}OO$. ^{18}OOO and ^{17}OOO in Band C are relatively easy to retrieve because their spectral lines are positioned independently with other lines, but ^{18}OOO and $O^{17}OO$ in Band B are positioned at the shoulder of the intense spectral lines of O_3 and HCl respectively, so retrieval results of those isotopes are likely to be affected by O_3 and HCl results.

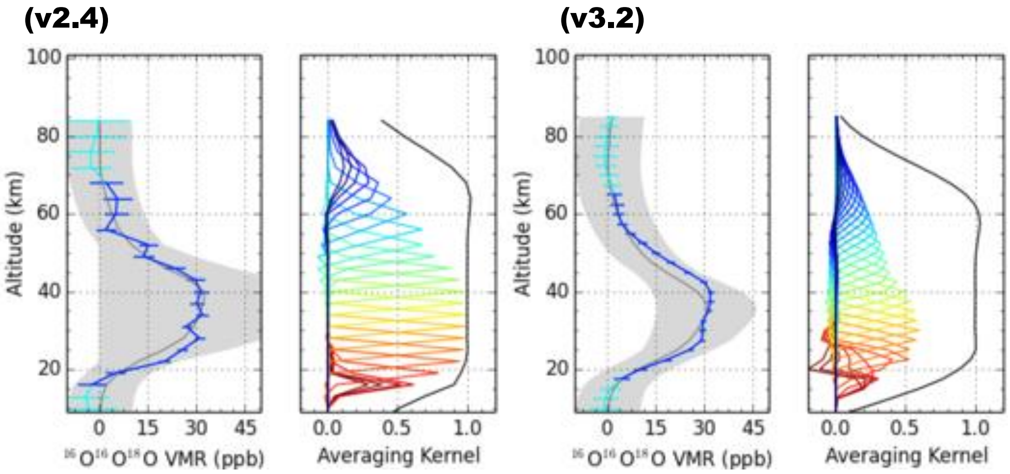

Figure 3.3-20 ^{18}OOO (band C) as in Figure 3.3-1.

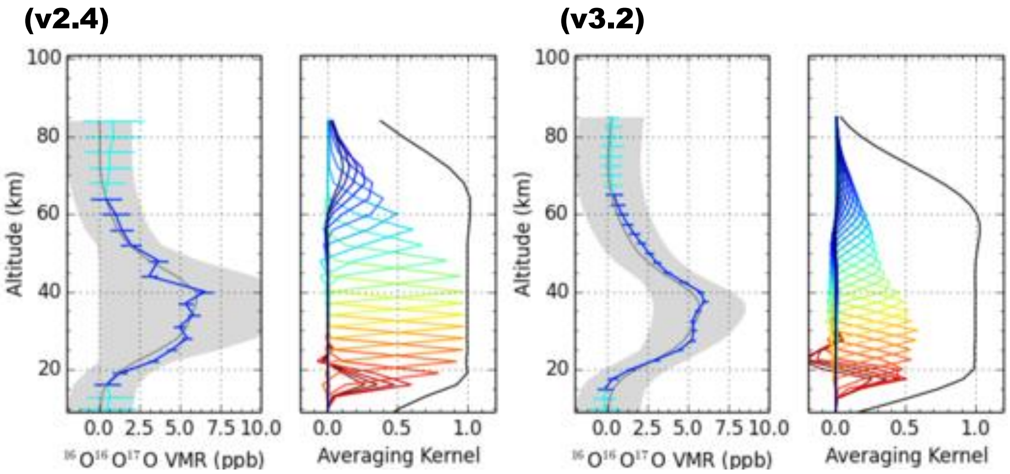

Figure 3.3-21 ^{17}OOO (band C) as in Figure 3.3-1.

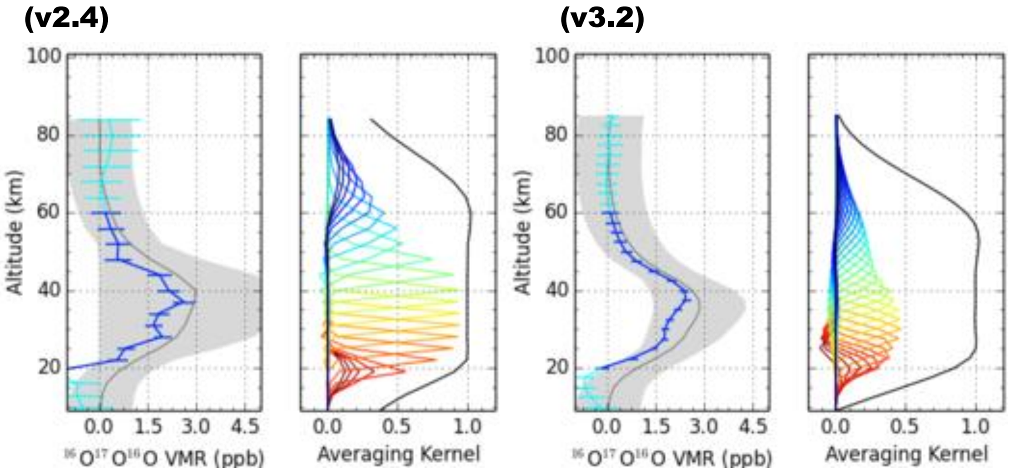

Figure 3.3-22 $O^{17}OO$ (band B) as in Figure 3.3-1.

3.4. Remaining Issues

- The Dicke narrowing effect was not considered and the profiles in the upper mesosphere may have negative bias. However, we have found that this effect is small in reality.
- Frequency calibration in L1 processing has long-term drift.
- Differences between profiles retrieved from AOS1 and AOS2 according to the revision of AOS response function. For O_3 and HCl in Band A, those differences are as high as around 5% in the mesosphere.

4. SMILES L2 PRODUCTS

4.1. DEFINITION OF DATA PRODUCTS

The definitions of datasets are in Table 4.1-1. The DPS-L2 produces Level 2 data to convert the calibrated measurements of brightness temperature called Level 1B data into vertical distributions of geophysical parameters along the measurement track of the instrument. The main geophysical parameters retrieved are in Table 4.1-2

Table 4.1-1 SMILES Datasets

Data type	Description
RAW	Unprocessed mission data in binary packets
Level 0	Reconstructed, unprocessed mission data in binary packets
Level 1B	Calibrated instrument radiances and related data
Level 2	Derived geophysical variables at the same resolution and location as Level 1 source data
Level 3 (not available)	Variables mapped on uniform space–time grid scales, usually with some completeness and consistency

4.2. L2 PRODUCTS OVERVIEW

There are two types of SMILES L2 products. One is “L2Product” and the other is “L2Product_G_RA”. The file names are defined as follows.

L2Product_G_RA:

SMILES_L2_{***product_name***}_{***version_name***}_{***observed_date***}.he5

L2Product:

SMILES_L2_{***product_name***}_{***band_name***}_{***version_name***}_{***observed_date***}.he5

“L2Product” includes all available datasets retrieved from all observation bands. Each file is separately provided by species, observed date and observation band. Data fields include *a priori* profiles, averaging kernels and retrieved profiles of the pressure grid (see Table 4.4-2). As a result, the size of each file is up to 8MB.

For “L2Product_G_RA”, each file is separately provided by species and observed date. For profiles retrieved with multiple bands, only the data from the band with higher “band priority” is provided. Data fields include only 5 items. As a result, the size of each file has been reduced to 0.8MB.

Table 4.2-1 Band priorities for each product

Product	Priority	Product	Priority	Product	Priority
O_3	A, B(, C)	HCl	B, A	ClO	C
HNO_3	C(, A)	HOCl	A	CH_3CN	A
BrO	C(, A)	HO_2	B, C	Temperature	A, B
^{17}OOO	C	$O^{17}OO$	B	^{18}OOO	B, C

4.3. DATA SCREENING

This version of the L2 product includes all the processed profiles but some of these are inadequate for scientific use. If using these profiles, we strongly recommend that usable scans are selected according to the following screening condition: *status* = 0 (for details, see Table 4.4-2). Moreover, L2 products include data for altitude range that is not usable for validation and/or scientific purposes.

If retrieval errors that include spectrum data information are not sufficiently smaller than errors without spectrum data, L2 profiles will be retrieved from other information (such as *a priori* profiles, smoothing effects of Tikhonov Regularization). In that case, these profiles should not be used in scientific analysis. In v2.4 algorithms, the threshold of effectiveness is set to 50%, and if retrieval errors exceed the threshold, the data in *L2Precision* field transforms into a negative value in order to notify data users.

4.4. PRODUCT FORMAT

We show the format of the HDF-EOS5 data file below.

Table 4.4-1 Structure of HDF-EOS5 data file

No.	Group	Attributes
1	***HDFEOS /SWATH /{product_name}***	Observation and retrieved data using retrieved altitude grids ・Retrieved profile ・Status flag ・Geolocation data and so on…
2	***HDFEOS /SWATH /{product_name}_Pressure***	Observation and retrieved data interpolated pressure grids
3	***HDFEOS/ ADDITIONAL/ FileAttribute***	File information such as: ・Instrument Name ・Processing Level ・Version ・Observation Day ・Band Name and so on…

*: http://www.hdfgroup.org/

(1) Standard processing data (HDF5-EOS)

The structure of standard processing data is as follows.

Table 4.4-2 Detailed structure of L2 product files
(Underlined fields are included in both types of L2 Product files)

Group/Dataset name	Explanation	Dimension	Type	Unit
HDFEOS				
SWATH				
{Productname}* [*1]				
Data Fields				
L2Value* [*2]	Retrieved Value	(nLevel,nTimes)	float	vmr
L2Precision	Calculation Error (negative values show unuseful data)	(nLevel,nTimes)	float	vmr
PrecisionWOsignal	Calculation Error without Signal Information	(nLevel,nTimes)	float	vmr
MeasurementError	Measurement Error	(nLevel,nTimes)	float	vmr
SmoothingError	Smoothing Error	(nLevel,nTimes)	float	vmr

Group/Dataset name	Explanation	Dimension	Type	Unit
Apriori	A Priori Value	(nLevel,nTimes)	float	vmr
AprioriError	A Priori Error	(nLevel,nTimes)	float	vmr
CorrLength	Correlative Length of A Priori	(nTimes)	float	km
AveragingKernel	Averaging Kernel	(nLevel,nLeveln Times)	float	-
VerticalResolution	Vertical Resolution	(nLevel,nTimes)	float	km
InformationValue	Information Value	(nLevel,nTimes)	float	-
Pressure	Retrieved Pressure	(nLevel,nTimes)	float	hPa
AprioriPressue (Temperature product only)	A Priori Pressure	(nLevel,nTimes)	float	hPa
Temperature (Except Temperature product)	Retrieved Temperature	(nLevel,nTimes)	float	K
WaterVapor	Using Water Vapor of Retrieval	(nLevel,nTimes)	float	vmr
Baseline0	Coefficient of Continuum	(nLevel,nTimes)	float	km^{-1}
Baseline0Precision	Baseline Error of Coefficient	(nLevel,nTimes)	float	km^{-1}
Baseline1	Primary Coefficient of Continuum	(nLevel,nTimes)	float	$Hz^{-1}.km^{-1}$
Baseline1Precision	Baseline Error of Primary Coefficient.	(nLevel,nTimes)	float	$Hz^{-1}.km^{-1}$
Baseline2	2nd Coefficient of Continuum	(nLevel,nTimes)	float	$Hz^{-2}.km^{-1}$
Baseline2Precision	Baseline Error of 2nd Coefficient	(nLevel,nTimes)	float	$Hz^{-2}.km^{-1}$
Baseline3	3rd Coefficient of Continuum	(nLevel,nTimes)	float	$Hz^{-3}.km^{-1}$
Baseline3Precision	Baseline Error of 3rd Coefficient	(nLevel,nTimes)	float	$Hz^{-3}.km^{-1}$
RadianceResidualMax	Max. Radiance Residual	(nTimes)	float	K
RadianceResidualMean	Mean Radiance Residual	(nTimes)	float	K
RadianceResidualRMS	RMS Radiance Residual	(nTimes)	float	K
RetrievedViewAngleOffset	Antenna Elevation Angle Offset	(nTimes)	float	degrees
RetrievedViewAngleOffsetError	Antenna Elevation Angle Offset Error	(nTimes)	float	degrees
NumIterPerform	Convergence Loop Number and Result	(nTimes)	int	-
MaxNumIteration	Max. Convergence Number	(nTimes)	int	-
Status	Status Information • Useful Data = 0 • Error Status Spectrum Fitting =1 Altitude Range =2 Convergence Status = 4 HCl Profile Status = 8	(nTimes)	int	-
SeqCount	Sequence Counter	(nTimes)	int	-
AOSUnitNum	Number of Observed AOS Unit	(nTimes)	int	-
Convergence	Convergence Status	(nTimes)	float	-

Group/Dataset name	Explanation	Dimension	Type	Unit
FOVInterference	Interference Flag ・ NO Interference = 0 ・ Interference by Sun = 1 / Moon = 2 / Solar Paddle = 4 ・ NO information = -1	(nTimes)	int	-
CostfunctionYAll	Cost/function of Spectra	(nTimes)	float	-
CostfunctionY	Cost/function of Spectra for each Altitude	(nLevel,nTimes)	float	-
DifferenceYAll	Maximum HCl Difference between Scan and Zonal Mean Profile normalized by std.	(nTimes)	float	-
DifferenceY	HCl Difference between Scan and Zonal Mean Profile normalized by std.	(nLevel,nTimes)	float	-
Geolocation Fields				
Time	Observation Time (Total no. of seconds since 1/1/1958)	(nTimes)	double	seconds
TimeUTC	Observation Time （UTC） yyyy-mm-dd hh:mm:ss.sss	(nTimes)	char	-
Altitude	Representative Altitude	(nLevel)	float	km
Latitude	Observation Latitude	(nTimes)	float	degrees
Longitude	Observation Longitude	(nTimes)	float	degrees
SolarZenithAngle	Solar Zenith Angle	(nTimes)	float	degrees
LocalTime	Local Time	(nTimes)	float	-
LineOfSightAngle	Azimuth View	(nTimes)	float	degrees
AscendingDescending	Ascending/Descending Flag (Asc = 0 / Desc = 1)	(nTimes)	char	-
Reserved	Reserved Field	(nTimes)	int	-
{Productname}_Pressure[*3]				
Data Fields				
L2Value	Retrieved Value	(nLevel,nTimes)	float	vmr
L2Precision	Calculation Error	(nLevel,nTimes)	float	vmr
RadianceResidualMax	Max. Radiance Residual	(nTimes)	float	K
RadianceResidualMean	Mean Radiance Residual	(nTimes)	float	K
RadianceResidualRMS	RMS Radiance Residual	(nTimes)	float	K
NumIterPerform	Convergence Loop Number and Results	(nTimes)	int	-
Status	Status Information ・ Useful Data = 0 ・ Error Status Spectrum Fitting =1 Altitude Range =2 Convergence Status = 4 HCl Profile Status = 8	(nTimes)	int	-
SeqCount	Sequence Counter	(nTimes)	int	-
AOSUnitNum	Number of Observed AOS Units	(nTimes)	int	-

Group/Dataset name	Explanation	Dimension	Type	Unit
Convergence	Convergence Status	(nTimes)	float	-
FOVInterference	Interference Flag • No Interference = 0 • Interference by Sun = 1 / Moon = 2 / Solar Paddle = 4 • No Information = -1	(nTimes)	int	-
CostfunctionYAll	Cost/function of Spectra	(nTimes)	float	-
DifferenceYAll	Maximum HCl Difference between this Scan and Zonal Mean Profile normalized by std.	(nTimes)	float	-
CostfunctionYAll	Cost/function of Spectra	(nTimes)	float	-
***InformationValueLimited* (**1)**	Integrated Averaging Kernel around target grid.	(nLevel,nTimes)	float	-
Geolocation Fields				
Time	Observation Time (Total no. of seconds since 1/1/1958)	(nTimes)	double	seconds
TimeUTC	Observation Time（UTC）yyyy-mm-dd hh:mm:ss.sss	(nTimes)	char	-
Pressure	Representative Pressure	(nLevel)	float	hPa
Latitude	Observation Latitude	(nTimes)	float	degrees
Longitude	Observation Longitude	(nTimes)	float	degrees
SolarZenithAngle	Solar Zenith Angle	(nTimes)	float	degrees
LocalTime	Local Time	(nTimes)	float	-
LineOfSightAngle	Azimuth View	(nTimes)	float	degrees
AscendingDescending	Ascending/Descending Flag (Asc = 0 / Desc = 1)	(nTimes)	char	-
Reserved	Reserved Field	(nTimes)	int	-
ADDITIONAL				
FILE_ATTRIBUTES* [*4]				
HDFEOS INFORMATION				
StructMetadata.0	Matrix Information for Swath Data	1	char	-
coremetadata.0	HDF-EOS Information	1	char	-

**1: Newly added field in v3.0 product

[*1] Attributes of {Productname} group

No.	Name	Explanation	Dimension	Data type	Unit
1	***Altitude***	Calculation Altitude	(nLevels)	float	km
2	***VerticalCoordinate***	Vertical Coordinate System Name	-	char	

*2 Attributes of Dataset in Geolocation/Data fields group

No.	Name	Explanation	Dimension	Data type
1	***MissingValue***	Missing Value	-	float
2	***Title***	Field Name	-	char
3	***Units***	Unit	-	char
4	***UniqueFieldDefinition***	Field Definition	-	char

*3 Attributes of {Productname}_pressure group

No.	Name	Explanation	Dimension	Data type	Unit
1	***Pressure***	Calculation Pressure	(nLevels)	float	hPa
2	***VerticalCoordinate***	Vertical Coordinate System Name	-	char	

*4 Attributes included File Attribute group

No.	Name	Explanation	Dimension	Data type
1	***L1BID***	L1B File Name	(nTimes)	char
2	***InstrumentName***	Instrument Name (SMILES)	-	char
3	***ProcessLevel***	Processing Level (L2)	-	char
4	***StartUTC***	Start Time for File (yyyy-mm-ddT00:00:00.000)	-	char
5	***EndUTC***	End Time for File (yyyy-mm-dd T23:59:59.000)	-	char
6	***GranuleMonth***	Month (mm)	-	int
7	***GranuleDay***	Day (dd)	-	int
8	***GranuleDayofYear***	Granule Day of Year	-	int
9	***GranuleYear***	Year (yyyy)	-	int
10	***PGEVersion***	Processing Version (XXX-XX-XXXX)	-	char
11	***StartScan***	Scan Count for First Day for File	-	char
12	***EndScan***	Scan Count for End Day for File	-	char
13	***BandName***	Band Name	-	char

4.5. BIAS DATA

There is a possibility that the SMILES measurement may include systematic biases arising from non-linear correction and uncertainty in line parameters. For the proper use of the SMILES data it would be suggested that such systematic errors should be removed as much as possible. We derived differences from the zonal mean values which are expected to be zero under specific conditions, and defined them as systematic biases. Detailed conditions for some atmospheric species are described in Table 4.5-1.

Table 4.5-1 Conditions for Bias Data

Species	Height range	Conditions	Remarks
ClO	~25km	Solar Zenith Angle > 113°	There is possibility that the bias is not properly estimated at 50-70°N during January and February 2010 owing to the distortion of polar vortex.
	28~34km	Solar Zenith Angle > 113° Local time 0 – 6h	
	68km~	Solar Zenith Angle < 83°	
BrO	~34km	Solar Zenith Angle > 113°	
	37~40km	Solar Zenith Angle > 113° Local time 0 – 6h	
	56km~	Solar Zenith Angle < 83°	
HO2	~32 km	Solar Zenith Angle > 113°	
	36~40km	Solar Zenith Angle > 113° Local time 0 – 6h	
HOCl	56km~	Solar Zenith Angle < 83°	

* Settings for AOS thermal control heater were changed on 24/10/2009 and 27/10/2009.

Since the systematic biases differ under the specific conditions, such as measurement bands, instrument states, and latitude, we derived them for each.

Data files containing the systematic biases are provided to users as a part of the product data after v3.0. The definition of file names is as follows.

SMILES_L2_bias_{***product_name***}_{***band_name***}_{***version_name***}_AU{***num***

ber_of_AOS_units}_{***latitude***}.dat

Ex) SMILES_L2_bias_BrO_A_AU1_008-11-0502_-10.0.dat

The following output is an example of the systematic biases. If the bias is not calculated because of missing data, a missing value -999.99 is filled; if the height range is out of derivation, '0' is filled in the data file.

```
# BrO bias
# Version 008-11-0502
# Band A
# AOSUnitNum 1
# Latitude range S05-N05
# altitude bias (vmr)
# (km)   1012-1023   1024-1026   1027-1031   1101-1130   1201-1231   0101-0131   0201-0228   0301-0331   0401-0421
8.0      5.0000e-10  5.0000e-10  5.0000e-10  5.0000e-10  5.0000e-10  5.0000e-10  5.0000e-10  5.0000e-10  -999.99
10.0     2.0132e-10  2.0132e-10  2.0132e-10  2.0132e-10  2.0132e-10  2.0132e-10  2.0132e-10  2.0132e-10  -999.99
12.0     9.0243e-09  9.0243e-09  9.0243e-09  9.0243e-09  9.0243e-09  9.0243e-09  9.0243e-09  9.0243e-09  -999.99
…        …           …           …           …           …           …           …           …           …
84.0     9.0243e-03  9.0243e-03  9.0243e-03  9.0243e-03  9.0243e-03  9.0243e-03  9.0243e-03  9.0243e-03  -999.99
```

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Appendix

A. 1. Information in the previous versions

A. 1. 1. Description of v1.0 (005-06-0024)

V1.0 is a test version in order to check L2 processing algorithms designed before launch (Takahashi et al., 2010). V1.0 gave priority to quality rather than quantity and 46 % of L1B files which had some kind of error status were not processed.

- The tangent altitude (geometrical) is calculated by using a) SMILES Star Sensors, b) SMILES scan mirror angle, and c) ISS position. SMILES Star Sensor shows unexpected large scattered output. We smoothed out the SMILES tangent altitude by second order fitting in this version. The tangent altitude precision should be 100 m (1 sigma) in rms according to the specifications which are now under verification.
- The two SMILES Star Sensors are pointing in fairly close directions to each other therefore there is a possibility that the SMILES tangent point cannot be calculated when both the sensors are within 45° of the Sun. In this situation, no L2 product is processed.
- The condition of vertical correlation is not introduced in the retrieval of any species except temperature, according to the results of the vertical correlation study.

A. 1. 2. Improvements in v 1.1 (005-06-0032) update

The goal of v1.1 is to increase the amount of useful data for creating gridded data using STT-ISS hybrid pointing data.

- The pointing direction for determining tangent altitudes is calculated by using SMILES scan mirror angle and ISS position. However, since pointing accuracy will heavily affect tangent altitude determination errors and an average altitude within a single scan is retrieved using the SMILES Star Sensor in L2 processing. In the case that sunlight or moonbeams enter the FOV of the SMILES Star Sensor, positioning information cannot be obtained, so this will be estimated from the information of 50 scans before and after the scan in question.

A. 1. 3. Improvements in v 1.2 (005-06-0150) update

The goal of v1.2 is to suppress internal inconsistency between receivers. SMILES has 2 receivers (units 1 and 2) and response functions are fitted with the sum of triple-Gaussian functions based on ground test data. However, these functions are not correct and mesospheric O_3, HCl and temperature have differences of 10-20 % between receiver units 1 and 2. We include experimental correction factors for the functions which determine that retrieved temperatures agree with TIMED/SABER.

- Illegal values in longitude when the longitude of the tangent point is around 180 degrees have been corrected.
- Altitude offset of Star Trackers (STT) has been reduced to +/- 1km due to the implementation of a compensation formula for time from STT.
- Rate of convergence in the retrieval process has been improved by smoothing vibrations in the ISS altitude data which do not seem to represent actual vibrations.
- Description of line shape has been refined with introducing the coefficient (v/v_0) .
- Line parameters of O_3, HNO_3, HO_2 and ozone isotopes have been changed from the JPL catalog to HITRAN2008.
- Profiles of temperature and HCl around 50km have been improved, with the compensation of an effect from the Doppler shift.
- Consistency between retrieval results from Band A in Setting 2 (Bands A/C) and Setting 3 (Bands B/A) have been improved by compensating between the response functions of AU1 and AU2 (2 units in AOS).
- Hydrostatic assumption has been introduced as a constraint in the calculation of pressure and temperature.
- Retrieval results of HOCl have been improved by ignoring ozone isotopes whose absorption lines overlap that of HOCl in Band A.
- Information contents of ozone isotopes, HNO_3, ClO and CH_3CN have been increased by adjusting the error value in the *a priori* profile.
- Rate of convergence in the retrieval process has been increased by ignoring temperature retrieval in Band C.
- Rate of convergence in the retrieval process has been increased by raising the upper limit of iteration trials in the retrieval process from 5 to 8.

A. 1. 4. Improvements in v 1.3 (006-06-0200) update

In this version, determination of screening flags and overall algorithm have been slightly modified. Mainly changes that have a physical basis have been adopted as it is assumed that these modifications can significantly affect the retrieved profiles with the implementation of the next planned update of L1B data processing.

- L1B data has been updated from version 005 to version 006.
- Retrieved profiles from scans near "FOV interference" were improved by referring to "the flags indicating FOV disturbance." For details of the L1B data update, see the document "Level 1 Product Release Notes (Ver.006)".
- Standard temperatures for Lorentz width of absorption lines of O_3, HNO_3, HO_2 and ozone isotopes have been corrected from 300K to 296K. The effect of this correction is around a few percent.
- In correcting the tangent height on the observation point, antenna elevation offset introduction is retrieved from the average of altitude offset within one scan. According to this change, amounts of O_3 and HCl above 50km increase by a few percent.
- Antenna movement within the time to acquire a spectrum for single height is taken into account with the antenna pattern. This improvement causes an increase of a few percent in ozone at the peak height (lower stratosphere).
- In order to make better fitting of the curved baseline of brightness temperature, the uncertainty of absorption coefficient is fitted with a 2-dimensional function instead of its original 1-dimensional function. As a result, baseline residue has been decreased by around half in comparison with the previous version.
- Regularization of status vectors in the inversion model with a priori errors has been introduced. Due to this improvement, 2-dimensional terms of the absorption coefficients with a small number of digits can be retrieved.
- The grids of retrieval altitude have been adjusted by 2, 3 or 4 km depending on species, band and altitude, instead of the uniform 3 km in the previous version. In adjusting the altitude grid, the information of altitude resolution is referred to. As a result of this modification, species with high sensitivity (such as O_3 and HCl) can be retrieved on a more precise altitude grid, and those with low sensitivity (such as BrO and HO_2) can be retrieved with a wider altitude range.
- Altitude correlation of 10 km has been introduced for all species except O_3 from Bands A and B.
- Information on convergence, FOV interference and observation altitude are stored in the *status* field. For details, see the format sheet in the Product Guide of v1.3.
- Information in order to evaluate spectrum residue, cost function for all species and all altitudes is stored in the *CostFunctionY* and *CostFunctionYAll* fields in the products.

- Bugs in the *AveragingKernel*, *InformationValue* and *VerticalResolution* fields have been fixed.
- Preliminary "status flag" has been newly added from this version onwards.
- For the retrieval of Band C, a priori values for the tangent altitude are provided from Bands A or B. (There are operational modes with Bands A+C and Bands B+C.)

A. 1. 5. IMPROVEMENTS IN V 2.0 (007-08-0300) UPDATE

The objective of this update is to improve temperature profiles. L1B data has been updated to version 007 in which non-linear correction has been newly implemented. In this version, biases in stratospheric temperature have been suppressed and therefore O3 amounts decreased by 8% at the peak altitude. [Mitsuda et al., 2011]

- L1B data has been updated from version 006 to 007.
- Gain nonlinearity correction has been applied to observed spectra (Ochiai et al., 2012). In the middle stratosphere, retrieved temperatures become closer to those of the Goddard Earth Observing System-5 assimilated data. Nonlinearity effects influence not only temperature but also other molecules. For those species such as O_3, HCl and ClO with strong lines the retrieved values decrease by 5- 7% at 25- 45 km. For those species such as HOCl and BrO with weak lines located at the wing of strong lines, the retrieved values change from around 50- 100 %. In v1.3, the retrieved profiles of HOCl contained negative values at around 30km, but this has now been improved.
- A new AOS response function has been introduced. This function was modeled on new on-orbit measurement data for AOS response function in January of 2011 (Ozeki et al., 2011).
- Temperature field in the mesosphere is very sensitive to retrieval results, but retrieved temperature profiles above 40- 50 km were not so good. Thus MLS temperature products (v2.2) to which the migrating tidal model (Global Scale Wave Model) was applied were referred to as the mesospheric temperature field.
- Preliminary corrections in observed frequency grids have been introduced. By removing frequency fitting residue in L1B data, residue in general decreases from 100 kHz to 50 kHz.
- Some line parameters have been updated.
- Bugs in frequency grids around $O^{17}OO$ (Band B) and ^{18}OOO (Band C) have been fixed. This update reduces systematic errors above 50km.

A. 1. 6. IMPROVEMENTS IN V 2.1(007-08-0310) UPDATE

The HOCl product was improved in v2.1. Other products such as O_3 have not been changed.

- Some line parameters have been updated. HOCl spectral lines are located at the shoulder of these lines. Residual spectra around HOCl were suppressed.

A. 1. 7. IMPROVEMENTS IN V 2.2 (007-09-0400) UPDATE

The objectives of this version are improvements in retrieval in the mesosphere and vibrations in the profile. In order to resolve these problems, the followings have been adopted.

- Altitude range of retrieval has been extended. In addition, the altitude ranges are independently modified by species (e.g. Upper limit of retrieval was 85 km for all species in the previous version but it has been extended up to 100 km for O_3, HCl and HO_2 whose sensitivity is relatively high). Moreover, *a priori* errors for BrO, $HO_{2,}$ and O_3 isotopes have been widened in comparison to the previous version. This has resulted in the presence of an HO_2 peak in the lower thermosphere at night-time.
- The inversion algorithm has been modified in order to suppress vibrations in the profiles. For the retrieval of O_3, HCl and HNO_3, Tikhonov Regularization has been implemented in combination with the Optical Estimation Method. (Manago et al., 2013)
- AOS response function has been revised. Although the data referred to in the retrieval process is still that of the same orbit as the previous version, another analytic method for modeling weaker signals has been adopted. (Mizobuchi et al., 2012)
- Spectral line parameters for O_3 and its isotopes have been modified. The preliminary results of a new measurement experiment have been replaced with certified values. For ^{18}OOO in Band B, the parameters have been also replaced from HITRAN2008 [*Rothman et al.*, 2009] with JPL Catalog [*Pickett et al.*, 1992]. As a result, the spectrum residual has been significantly improved.
- Some other minor changes have been implemented:
  - For a priori profiles of HOCl, climatological data generated from Aura/MLS v2.2 has been replaced with CCSR/NIES climatological data.
  - A formula for gravity acceleration in the Forward model has been modified so

that the Geodetic Reference System 1980 has been adopted uniformly in the L2 retrieval system.

– For altitudinal interpolation of pressure data in *a priori* datasets, a linear interpolation of logarithm of pressure has been adopted instead of a linear interpolation of pressure.
– Some programming bugs have been fixed, such as mistakes in standard temperature for spectral line parameters of HCl.

A. 1. 8. Improvements in v 2.3 (007-09-0402) update

In this version, the retrieval algorithm is the same as that of v2.2, and some product data and flags have been improved.

- Datasets which interpolated with pressure grid data have been added. This grid data is uniform throughout all species.
- The definition of status flag has been modified and therefore that percentage of available scan data has exceeded 80% for all observation bands. Screening with convergence conditions has been relaxed, while screening with spectrum fitting has been newly introduced. Quality information for HCl profiles has been reflected in status flags for indicating FOV interference, instead of flags of FOV interference from L1B data. Quality information will have error values if an HCl profile runs out of variance for profile zonal means 5 times.

A. 1. 9. Improvements in v 2.4 (008-11-0502) update

The objectives of this version are improvements in thermospheric O_3 and HCl and mesospheric HCl. The following items have been adopted.

- Extension of height range (O_3, HCl, HO_2, BrO): In v2.1 retrieval height range was set at 8-85 km for all parameters, but in this version the upper limit for retrieval height range is set at 120 km for O_3 and at 100 km for HCl and HO_2. At the same time a priori values and their errors are adjusted for better comparison with other data sources, resulting in improvements for those species. In addition, after adjusting a priori errors for BrO, it is possible to evaluate biases between day-time and night-time values.
- Smoothing profiles (O_3, HCl, HNO_3): In v2.1, some oscillations remained to the order of a few percent at 50 km for O_3 and HCl profiles, and there was divergence of HNO_3 profiles in the lower stratosphere. To reduce these erroneous behaviors we applied the Tikhonov Regularization Method (TRM) in addition to the ordinal

Optimal Estimation Method (OEM) for the L2 inversion algorithm. We also use the updated AOS response function prepared by the SMILES instrument team [Mizobuchi et al., 2013]. All these improvements contribute to reducing mesospheric O_3 and HCl oscillations.

- Increase in available data: The number of usable profiles increases by investigating screening conditions. So far we have included quality flags for L1B data and status of L2 profile convergence, but due to field obstacle flags, about 20% of data for one of the L1B data quality flags was judged to be inappropriate for use. In addition, we looked into variations in state vectors normalized by random errors as the threshold to observe the validity of retrieval results; however, the threshold is no longer appropriate since theoretical errors become smaller after introducing the Tikhonov Regularization Method. In v2.4, consistency seen in HCl profiles is used for the new screening conditions. Among species that have strong line intensity such as O_3, HCl, and ClO, HCl measurements were done at all times and as its diurnal and seasonal variations are relatively small, we decided to utilize the HCl data for evaluating the quality of retrieved profiles. Moreover, we have included the fitting residual as one of the quality flags, as the residual becomes valid when using the Tikhonov Regularization Method.
- L1b data has been updated to version 008. In this version, non-linear correction factors and information for tangent height have been revised (Ochiai et al., 2012).
- *A priori* and its errors for O_3 and HCl have been modified in order to extend the available altitude range for retrieval process up to the lower thermosphere.
- GEOS-5 dataset, which is used as an a priori for the meteorological field, has been revised by nudging with temperature and O_3 data from MLS observation, which resulted in the improvement of mesospheric temperature in the dataset. For the *a priori* of temperature profiles in the v2.4 algorithm, GEOS-5 is referred up to 70 km, and the nearest grid of Aura/MLS data is referred to at a higher altitude. Tidal correction of Aura/MLS data with GSWM has been suspended. As a result of these modifications, the variance of mesospheric HCl which depends on temperature variation has been suppressed.
- The frequency of spectral lines of O_3, excited O_3 and O_3 isotopes have been re-measured in laboratory experiments (Ozeki, *private communications*). As a result of this modification, the peak amount of HOCl has changed by around 10%, whose spectral line is positioned at the shoulder of these O_3.
- For *a priori* profiles, climatological data from UARS/MLS data has been replaced with the calculation results from the nearest grid from SD-WACCM.

A. 1. 10. Improvements in v 3.0 (118-12-0602) update

In this version, the retrieval algorithms are modified to reduce the difference between AOSs and to improve retrieved values of species with weak signals.

- Calibrated brightness temperature (Level 1B processing): L1B product has some problems about the correction of non-linearity in brightness temperature calibration. In second-latest L2 product (v2.4), which used the latest L1B product (v008), difference of profiles of O_3 and HCl between the AOSs had increased, especially in the data observed in October, 2009. So we produced another L1B product (v118), in which brightness temperature is same as second-latest L1B product (v007). The v3.0 has been produced based on L1B v118 product.
- Inversion model: In the previous version, O_3, HCl, HNO_3 had been retrieved with the combination of Optimal Estimation method (OEM) and Tikhonov Regularization method (TRM) Level 1, while other species had been retrieved with only OEM. For the v3.0 product, the combination of OEM and TRM level 2 is applied for retrieval of all species. In addition, for HOCl profiles (which the vibration is large) and HNO_3 (band C) profiles (whose vibration negatively affect to BrO profiles), larger regularization factors are applied.
- The following has been modified in the inversion model with introduction of the TRM:
  - Altitude grid for retrieval is set to 2.5km for all species.
  - Altitude correlation of OEM is set to 0.01km for all species.
  - Climatology data of SD-WACCM (Specified-Dynamics WACCM) is used as a priori data for all parameters except meteorological values. (See Table 2.5-2)
  - The value of integral of averaging kernel within +/- 5km of target altitude grid has been newly adopted the criterion for determining of “useful altitude range”, with whose threshold set to 0.6. Users can screen the useful altitude range with the criteria “***L2Precision*** < 0”, which is not changed from the previous products.
- Modification in the product format: ***InformationValueLimited*** is newly added to the product HDF field, which means the value of integral of averaging kernel around +/- 5km of target altitude grid.

- Bias data for ClO, BrO and HO_2: In addition to profile data for each species, night-time bias data for ClO, BrO, HO_2 are released as ancillary data. See the Product Guide (v2.4) for details of retrieval method of the bias.

A. 1. 11. Improvements in v 3.1 (118-12-0612) update

In this version, in addition to v3.0 the retrieval algorithms are modified to reduce the difference between AOSs and to improve retrieved values of species with weak signals. The number of scans in the product increases 0.3%.

A. 1. 12. Improvements in v 3.2 (118-12-0702) update

In this version the retrieval algorithms are improved to reduce random errors of O_3, HCl, and HO_2 in the mesosphere.

- Inversion model: We found stronger oscillations of retrieved profiles in v3.1 than v2.4. Therefore, we applied larger regularization factors to reduce the oscillation. In particular for HNO_3 (Band C) we used much larger regularization factors than other species since errors in HNO_3 would cause negative influence in retrieving BrO profiles
- Changes in a priori and a priori error profile: We looked again at a priori and a priori error profile to reduce oscillations in O_3, HCl, HO_2 in the mesosphere.

A. 2. Sample of source code for reading L2 product (in python)

A sample python code is shown below.

```
#!/usr/bin/env python

# import normal libraries.
import os
import sys
import numpy as np

# import HDF5 library
import h5py

print "Process Start   ---------------------"

# set HDF file
fnam = 'dir/008-11-0502/A/2009/10/12/SMILES_L2_O3_A_008-11-0502_20091012.he5'

# open HDF file
if os.path.exists(fnam):
    f = h5py.File(fnam,'r')
else :
    print 'File does not exist: %s'%(fnam)
    sys.exit()

# read HDF fields
L2Val=np.array(f['/HDFEOS/SWATHS/O3/Data Fields/L2Value'])
L2Prc=np.array(f['/HDFEOS/SWATHS/O3/Data Fields/L2Precision'])
L2Flg=np.array(f['/HDFEOS/SWATHS/O3/Data Fields/Status'])
L2Tim=np.array(f['/HDFEOS/SWATHS/O3/Geolocation Fields/Time'])
L2Alt=np.array(f['/HDFEOS/SWATHS/O3/Geolocation Fields/Altitude'])

# change array's shape (timexaltitude)
L2Val=L2Val.reshape(len(L2Tim),len(L2Alt))
L2Prc=L2Prc.reshape(len(L2Tim),len(L2Alt))

# set scan screening condition
cnd = (L2Flg == 0)

# scan loop (screened)
for i in range(len(L2Tim[cnd])) :

    print 'LOOP %i -----------------------------'%(i)
    # print L2 data and precision.
    # However, if this data is unuseful, print "-999.99".
    for j in range((len(L2Alt))) :
```

```
        if ( L2Prc[i,j] < 0 ) :
            print L2Alt[j], '-999.99', '-999.99'
        else :
            print L2Alt[j], L2Val[i,j], L2Prc[i,j]

    # loop break
    if  i > 3 :
        break

print "Process end      ---------------------"
```