EARLY RESULTS FROM 4K-COOLED SUPERCONDUCTING SUBMM WAVE LIMB EMISSION SOUNDER SMILES ONBOARD ISS/JEM

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ABSTRACT:

Early comparison of O_3, HCl, and HNO_3 L2 products (ver. 005-06-0032) of the Superconducting Submillimeter-Wave Limb-Emission Sounder (SMILES) onboard International Space Station has been conducted. Good agreements are observed among SMILES, SVISAT-1/ACE-FTS, AURA/MLS, and ENVISAT.MIPAS, for O_3 and HCl below 45 km. SMILES HNO_3 profiles are statistically ~20% higher than ACE-FTS and MIPAS. At higher altitude region, 45-60 km, SMILES O_3 and HCl are considerably different from ACE-FTS and/or MLS. It is concluded, although future data updates will be necessary, SMILES O_3 and HCl below 45 km are both useful for scientific application with special cautions to the SMILES data quality.

1. INTRODUCTION

The Superconducting Submillimeter-Wave Limb-Emission Sounder (SMILES) (Mauko et al., 1997, Inatani et al., 2000, SMILES Mission Team, 2002) is one of the early science program onboard Japanese Experimental Module/Exposed Facility (JEM/EF) of the International Space Station (ISS). SMILES has been developed jointly by JAXA and NICT. SMILES measures Earth's limb in the 625-650 GHz frequency region by using 4-K cooled Superconductor-Insulator-Superconductor (SIS) junction device, which results $T_{sys} \simeq$ 400K and $NE\Delta T \simeq$ 0.4 K, i.e. 10 times higher sensitivity compared to previous limb atmospheric measurements in the mm/submm wavelength region, such as AURA/MLS (Waters et al., 2006) and ODIN/SMR(Frisk et al., 2003).

SMILES can measure several key species related to chemistry of O_3 layer; O_3 (O_3, ^{17}OOO, $O^{17}OO$, ^{18}OOO, and $O^{18}OO$), HCl ($H^{35}Cl$ and $H^{37}Cl$), ^{35}ClO, HO_2, $HO^{35}Cl$, ^{81}BrO, and CH_3CN. The 350-400 km and 52° inclined ISS orbit shows 88-90 days precession period, which means that SMILES can measure diurnal variation of ClO, HOCl, HO_2, BrO and mesospheric O_3 within 45 days observation. The high sensitivity (T_{sys} ~ 400 K) and diurnal variation of the SMILES should open opportunity to investigate details of photochemistry of stratosphere and mesosphere which have not been investigated well before.

Profiles of SMILES data (O_3, HCl, etc), i.e. Level 2 (L2) data, are expected to have better precision (smaller error bar) compared to previous satellite measurements, because of better T_{sys} (~400K) and $NE\Delta T$ (~0.4 K) of the SMILES instrument. Accuracy of SMILES L2 data may not be as good as its precision, due to many reasons; such tangent height determination (Verdes, 2002; Takahashi et al., 2010), poor knowledge on instrument characteristics, uncertainty of spectroscopic errors (Verdes et al., 2005A and 2005B), approximations of algorithms, etc. The SMILES L2 dataset must be validated by comparing with existing dataset before the science application, especially coincidence comparison with satellite dataset, which have been already validated each other and they have good statistical coverage both in space and time.

In this paper we will introduce overview of SMILES instrument and Level 2 (L2) product (ver.005-06-0032) and some early verification results of O_3, HCl, and HNO_3 by comparing the coincidence events and the coincidence statistics with on-going satellite programs SCISAT-1/ACE-FTS, AURA/MLS, and ENVISAT/MIPAS. And accuracy of the SMILES dataset are discussed based upon the inter-satellite comparison.

2. SMILES OBSERVATION

SMILES was launched on Sep. 11, 2009 as a cargo payload of H-II Transportation Vehicle (HTV) by using H-IIB launcher from Tanegashima Space Center. SMILES have been operated from Oct. 12, 2009 to Apr. 21, 2010 when the submm local oscillator of the SMILES aborted operation.

Orbit characteristics of the ISS is 350-400 km in altitude and 52° inclination. Attitudes of ISS have varied frequently as much as ± 5° for pitch, yaw, and roll angles due to docking/undocking and other events.

SMILES (Kikuchi et al., 2010, and references therein) consists of (1) Scanning Antenna, (2) Single Side Band (SSB) Separator,

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(3) Local Oscillator, (4) SIS mixer, and (5) Acousto-Optic Spectrometer (AOS). SMILES observes 45° left from the forward direction of the ISS, which results nominal geographical coverage 38°S-65°N. Scanning antenna covers -30 to +160 km altitude region at tangent points. The observation cycle is 53s; the first 29.5 s is atmospheric measurement of ~2 km altitude interval at the tangent point in 0.5 s step. after the 29.5 s, the antenna was scanned quickly to the 160 km for the cold sky calibration. Internal room temperature hot load calibration and the frequency calibration have been carried out at every 53 s observation period. Details of instrument are already described in SMILES Mission Plan (JAXA and NICT 2002) and other (Kikuchi 2010),. Table 1 lists major characteristics of the SMILES system.

Frequency coverage	Band A (624.32 – 625.52 GHz) Band B (625.12 – 626.32 GHz) Band C (649.12 – 650.32 GHz)
Freq. sampling	0.8 MHz
Freq. resolution	1.8 MHz (FWHM)
System noise temp.	350~400 K in orbit
Integration time	0.5 s for each obs. tangent point
Noise tquivalent brightness temperature	~ 0.4 K in orbit
Calibration accuracy	< 1.0 K (specification)
Obs. cycle	53 s
Obs. alt. range	0 - 160 km
Vertical sampling	~2 km *(nominal)*
Instrumental vertical resolution	3.5 - 4.1 km *(nominal)*
Latitude coverage	38°S - 65°N *(nominal)*

Table 1. Characteristics of SMILES instrument.

3. SMILES L2 DATA

3.1 L2 Processing Algorithm

The retrieval algorithm (Takahashi et al. 2010; Imai et al., 2010) of operational L2 processing system is based on the OEM applied for atmospheric sounding (Rodgers, 1976). The maximum a posteriori estimate can be derived from statistical combination of a priori knowledge of a state vector $\boldsymbol{x}$ and the information on the measurement. We use a modification of the Gauss-Newton method called the Levenberg-Marquardt method (Levenberg, 1944; Marquardt, 1963). The retrieved state vector $\boldsymbol{x_{i+1}}$ at the iterative step i+1 is calculated as

$$x_{i+1} = x_i + \left(K_{xi}^T S_y^{-1} K_{xi} + S_a^{-1} + \gamma D\right)^{-1} \left\{K_{xi}^T S_y^{-1}\left[y - F\left(x_i, b\right)\right] + S_a^{-1}\left(x_i - x_a\right)\right\}, \tag{1}$$

where, $\boldsymbol{x}$ is a state vector of length $\boldsymbol{n}$, which contains concentrations of the species, atmospheric temperature, and pointing offset. The $\boldsymbol{y}$ is a measurement vector of length $\boldsymbol{m}$, which denotes the calibrated brightness temperature observed by the SMILES, and $\boldsymbol{F}$ is a forward model including both atmospheric radiative transfer and instrument characteristics. ***A priori*** knowledge is represented by the expected state $\boldsymbol{x}$ and its covariance matrix $\boldsymbol{S_a}$. $\boldsymbol{S_y}$ is the covariance matrix of $\boldsymbol{y}$. The matrix $\boldsymbol{K_{xi}}$ is a weighting function for each of the retrieval parameters evaluated at $\boldsymbol{x_i}$. The $\boldsymbol{x_a}$ normally corresponds to the initial guess $\boldsymbol{x_0}$, $\boldsymbol{D}$ is a scaling matrix that is usually assumed to be $\boldsymbol{S_a^{-1}}$, and γ is a Levenberg-Marquardt parameter which is initially set to 10^{-3} in the released two datasets (vers. 005-06-0024, and 0032), respectively.

A priori value and their covariance have been prepared from monthly zonal mean (10° latitude bin) of Aura/MLS. Initial value of temperature, humidity, and pressure are meteorological data provided by NASA/GSFC (6 hours interval) (Rienecker, M. M. et al., 2007).

In the present study, SMILES ver.005-06-0032 (here after ver. 0032) has been used. Major differences of the versions 0024 and 0032 from the algorithm theoretical basis document (ATBD) work (Takahashi et al., 2010) are initial tangent altitude guess. In the ATBD algorithm, initial tangent heights can be estimated within ±1km by using ancillary data. In the ver. 0024, initial tangent height is calculated from the smoothed value of Star Sensor of SMILES, and the line parameter of O_3, HCl are updated based upon the recent comparison (Perin et al., 2005). In the ver.0032, initial tangent heights are calculated using both Star Sensor of SMILES and the attitude data of ISS.

3.2 Expected Performance

Characteristics of retrieval results are mainly presented by an averaging kernel matrix $\boldsymbol{A}$, which is the sensitivity of the retrieved state to the true state, and a retrieval covariance matrix $\boldsymbol{S}$, whose diagonal elements shows the square of the retrieval precision. These are defined as follows:

$$A = \left(K_x^T S_y^{-1} K_x + S_a^{-1}\right)^{-1} K_x^T S_y^{-1} K_x, \tag{2}$$

$$S = \left(K_x^T S_y^{-1} K_x + S_a^{-1}\right)^{-1}. \tag{3}$$

In the non-linear case, these matrices are calculated by using the results of the final iteration process.

Eq. (3) means that, if target species have enough information, retrieval precision is depend almost on the S_y^{-1}. The S_y is calculated as square root of the noise equivalent brightness temperature, $NE\Delta T_B$,

$$\left(S_y\right)^2 = NE\Delta T_B = \frac{T_{sys} + T_A}{\sqrt{B\tau}}, \tag{4}$$

where the $\boldsymbol{T_{sys}}$ is the system noise in brightness temperature and the $\boldsymbol{T_{atm}}$ is the brightness temperature of the atmosphere, $\boldsymbol{B}$ is the receiver frequency bandwidth (2.1 MHz), and τ is the integration time (0.5 s). The $\boldsymbol{NE\Delta T_B}$ of the SMILES is ~ 0.4K, which is much better than 2.4 K (Odin/SMR) and 4.2 K (Aura/MLS) at the 600 GHz region. And SMILES should have better sensitivity in the measurements at the 600 GHz frequency region compared to the Odin/SMR and Aura/MLS.

Figure 1 shows the expected performance of the SMILES assuming the T_{sys} ~ 500 K (design target) for the mid-latitude atmosphere (Buhler et al, 2005; Takahashi et al., 2010; Kikuchi et al., 2011). In this estimation, covariance of *a priori*, $\boldsymbol{S_a}$, is assumed to be 100%, which means Error ratio S/S_a = 1.0 is equivalent to 100% error bar. O_3 and HCl can be retrieved <10% precision in the 20-65 km altitude range. Precision of HNO_3 retrieval can be expected better than 50% at the altitude region 20-35 km, but it can be improved by applying proper *a priori* restriction as described in the later section. Weaker species, such as BrO, can be retrieved ~ 50% in 30-40 km altitude range.

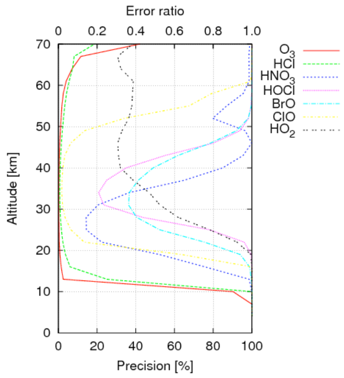

Figure 1. Theoretical retrieval precision of the target species, assuming 100% for S_a, which are O_3, HCl, HNO_3, HOCl, BrO, ClO, HO_2, retrieved from single-scan data in the daytime.

4. RESULTS

4.1 O_3 Products

Figures 2-4 show the example of O_3 retrieval at the coincidence with ACE-FTS ver.2.2 (Dupuy et al., 2009), Aura/MLS ver.2.2 (Froidevaux et al., 2008A), and ENVISAT/MIPAS MIPAS-IMK ver.40 (Von Clarmann et al., 2009), respectively. Altitude and value of O_3 maxima agrees well each other. Figures 5-7 show statistics of O_3 coincidence events at the 55°N-65°N latitude region. As clearly seen in Figures 6-8, SMILES O_3 at the 20-40 km altitude region agreed quite well (< 10 %) with ACE-FTS, Aura/MLS and ENVISAT/MIAPS (Dupuy et al., 2009; Froidevaux et al., 2008, Von Clarmann et al., 2009). This agreement was common for the all 10° latitude bins over 45°S-75°N. Above 40 km, SMILES O_3 showed 10% smaller value to the MLS and 30% smaller value to the ACE-FTS, respectively. It has been reported that the ACE-FTS O_3 tends to be 20% larger than other measurements at the 50-60 km altitude region. It can be concluded the statistical result shown in Figures 6-8 agree with previous works on the O_3 validation, and the SMILES O_3 value is 10% smaller to the mean of other observation.

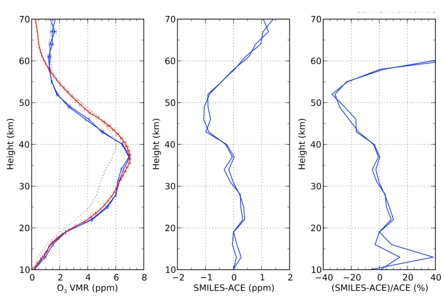

Figure 2. Example of O_3 coincidence; ACE-FTS ver.2.2 (Red) and SMILES (Blue) at latitude 66.0° and longitude 77.5°W on Nov. 13, 2009, profiles (left), absolute difference (middle), and relative difference (right). Two SMILESprofiles are compared with 1 ACE-FTS profile.

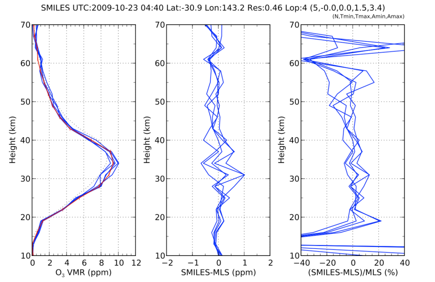

Figure 3. Example of O_3 coincidence; SMILES (red) and AURA/MLS ver.2.2 (Blue) at 30.9°S and 143.2°E on Oct. 23, 2009, similar to Figure 2. One SMILES profile is compared to 5 MLS profiles.

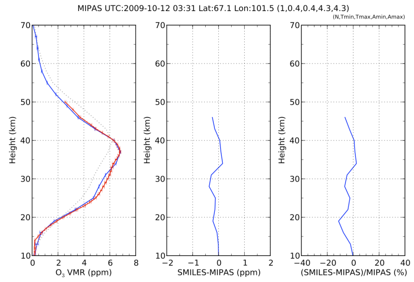

Figure 4. Example of O_3 coincidence; MIPAS-IMK (red) and SMILES (blue) at 67.0°N and 101.5°E on Oct. 12, 2009, similar to Figure 2.

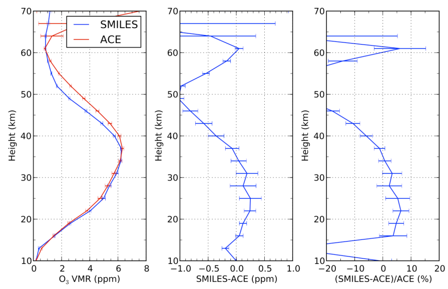

Figure 5. Statistics of 75 O_3 coincidences with 31ACE-FTS (ver.2.2) observations at the 55°N-65°N latitude region.

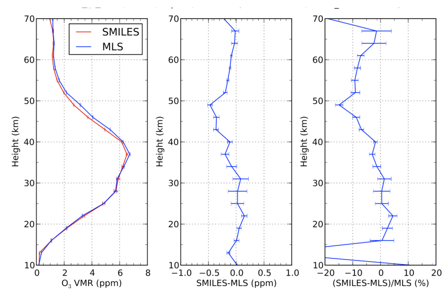

Figure 6. Statistics of 61 O_3 coincidences compared with 284 AURA/MLS (ver.2.2) observations at the 55°N-65°N latitude region.

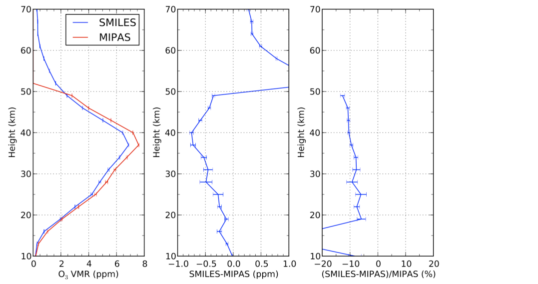

Figure 7. Statistics of 110 O_3 coincidences compared with 52 ENVISAT/MIPAS (MIPAS IML ver.40) observations at the 55°N-65°N latitude region.

4.2 HCl

Figures 8 and 9 show example of coincidences with ACE-FTS ver 2.2 (Mahieu et al., 2008) and MLS ver. 2.2 (Froidevaux et al., 2008B), respectively. Figures 10 and 11 show the coincidence statistics of SMILES compared with ACE-FTS and MLS in the 55°N-65°N latitude region, respectively. As similar to O3 coincidence statistics, SMILES HCl agreed quite well (< 5%) with ACE-FTS and MLS at 20-40 km altitude region. SMILES HCl value tends to be 20% smaller than ACE-FTS and MLS above 50 km. HCl should be ~ 3.5 ppb based upon observations and model studies, and SMILES HCl value (ver. 0032) above 40 km should not be used for science.

We think possible reasons that the SMILES HCl value to be too low (~3.0 ppb) above 50 km could be instrumental characteristics; such as, AOS frequency resolution, AOS frequency scaling, calibration, etc. And HCl value will be updated in the future release.

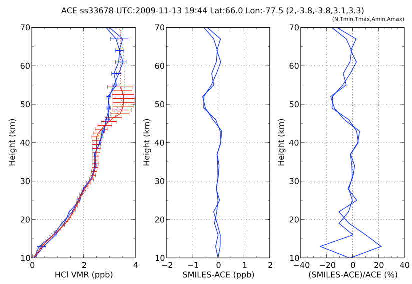

Figure 8. Example of HCl coincidence with ACE-FTS, at the event same as Figure 3.

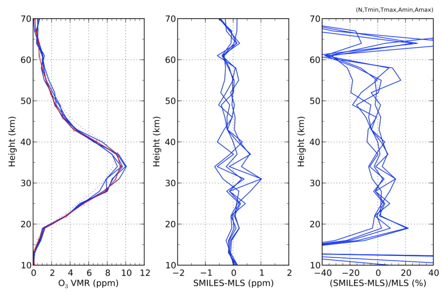

Figure 9. Example of HCl coincidence with AURA/MLS, at the event same as Figure 4.

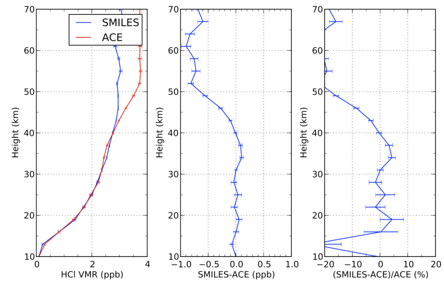

Figure 10. Statistics of HCl coincidence comparison with ACE-FTS at the 55°N-65°N region.

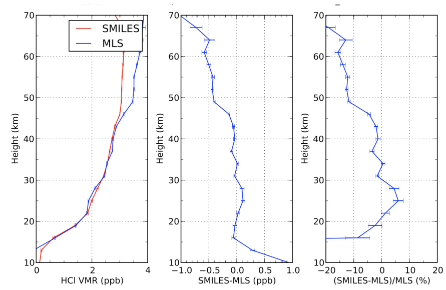

Figure 11. Statistics of HCl coincidence comparison with Aura/MLS at the 55°N-65°N region.

4.3 HNO_3

Figure 12 shows *a priori* used for the ver. 0032 processing and sample retrieval results. A priori is prepared from AURA/MLS ver.2.2 monthly zonal mean (Santee et al., 2007). MLS HNO_3 value is valid only up to 50 km, the retrieval error ***S*** clearly shows notch structure at the 50 km. By applying proper a priori constriction, we can retrieve HNO_3 properly even at 30-60 km altitude region.

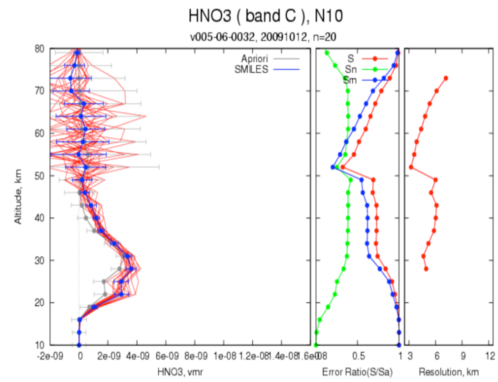

Figure 12. *a priori* used for the ver.0032 and retrieval results.

Figures 13 and 14 show the examples of HNO_3 coincidence with SCISAT-1/ACE-FTS ver.2.2 (Wolff et al., 2008) and ENVISAT/MIPAS, MIPAS-IMK ver.40 (Von Clarmann et al., 2009), respectively. Figures 15 and 16 show coincidence statistics at the 55°N-65°N latitude region. SMILES HNO_3 values are consistently higher, ~20%, than ACE-FTS and MIPAS. This is explained that the rotational quantum number dependence of pressure broadening parameter (Mencaraglia et al., 2006) is not used for the SMILES ver.0032. HNO_3 value of SMILES (ver.0032) and MLS (ver. 2.2) are quite similar since both do not include the rotational quantum number dependence of pressure broadening properly.

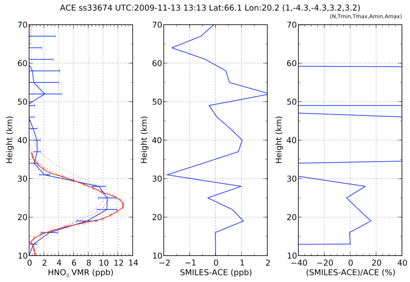

Figure 13. Example of HNO3 coincidence with SCISAT-1/ACE-FTS (ver.2.2) at 66.1°N, 20.2°E on Nov. 13, 2009. ACE-FTS HNO3 at the event of Figure 2 was not used since it showed non-convergence flag. One SMILES profile (red) is compared with MIPAS (blue).

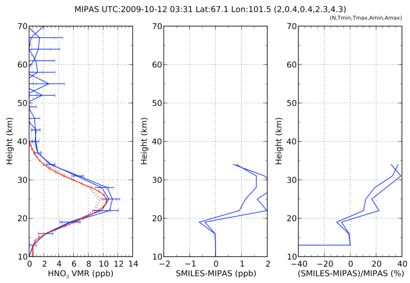

Figure 14. Example of HNO_3 coincidence compared with ENVISAT/MIPAS (MIPAS-IMK ver.40) at 67.1°N, 101.5°E on Oct. 12, 2009. Two SMILES profiles (blue) are compared with 1 MIPAS profiles (red).

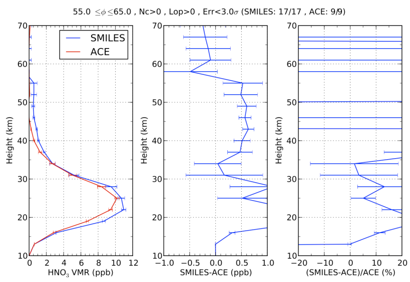

Figure 15. Coincidence statistics of SMILES HNO3 (ver.0032) compared with SCISAT-1/ACE-FTS (ver.2.2) at the 55°N-65°N latitude region. The 17 SMILES profiles are compared with 9 ACE-FTS profiles.

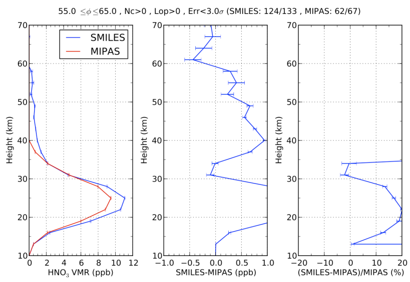

Figure 16. Coincidence statistics of SMILES HNO_3 (ver.0032) compared with ENVISAT/MIPAS (MIPAS-IMK ver.2.2) at the 55°N-65·N latitude region during Oct. 12-14, 2009. The 124 SMILES profiles are compared with 62 MIPAS profiles.

5. DISCUSSIONS AND SUMMARY

Tables 2-4 show summary of the coincidence statistics of O_3, HCl, and HNO_3, respectively. Statistics of O_3 profiles agree well among ACE-FTS, MLS, MIPAS and SMILES below 40km. The SMILES O_3 profile becomes statistically 30% lower than ACE-FTS (ver.2.2), and 10% lower than MLS (ver.2.2) and MIPAS-IMK (ver.40). It has been already reported that ACE-FTS O3 (ver.2.2.) shows 20% higher value compared with other observations including MLS (ver.2.2) and MIPAS (IMK ver.40). It is concluded that current SMILES O_3 value is 10% lower than other measurements. At the altitude region above 60 km, there is diurnal variation of mesospheric O_3, and we need more tight coincidence selection for the SMILES O_3 data validation.

Statistics of SMILES HCl profiles agrees quite well with ACE-FTS (ver. 2.2) and MLS (ver.2.2) below 45 km. Above 45 km, SMILES HCl profile becomes ~3.0 ppb, i.e. ~20% lower than the commonly agreed HCl value ~ 3.5 ppb.

This issue of SMILES O_3 at the altitude region 40-60 km and SMILES HCl above 45 km is under investigation. As shown in the Figures 8-11, SMILES HCl value above 40 km, ~ 3.0 ppb, is also 20% lower than the WMO recommendation, ~ 3.5 ppb. One possible explanation is spectral bandwidth of the two Acousto-Optical Spectrometer (AOS) have changed after the ground test, which was already confirmed by the on-orbit measurements.

Statistics of SMILES HNO_3 profiles is clearly 20% higher than ACE-FTS ver. 2.2 and MIPAS, IMK ver.40 as shown Figures 10 and 11. SMILES HNO_3 value is similar to MLS ver. 2.2 (the a priori value shown in Figure 12). This should be explained by the rotational number dependence of pressure broadening parameter of HNO_3, since the HNO_3 value of MIPAS have decreased ~20% by applying this rotational quantum number dependence (Mencaraglia et al., 2006).

We can conclude that SMILES O_3 and HCl data (ver. 005-06-0032) are scientifically useful below 45 km altitude region. SMILES HNO3 data should be updated before to be applied scientific works. SMILES L2 data updates to fix the issues discussed in the present work are already scheduled twice within the year 2010.

Altitude (km)	ACE-FTS	MLS	MIPAS
45~55	-20 ~ -30 %	-5 ~ -20%	-10 %
35~45	0~ -15 %	< ±5 %	< ± 5 %
25~35	< + 5 %	< ±5 %	< ± 5 %
<25	~ +5 %	< ±5 %	-10 %

Table 2. Results of coincidence statistics of SMILES O_3 (%) compared with ACE-FTS (ver. 2.2), MLS (ver. 2.2) and MIPAS (IMK ver.40).

Altitude (km)	ACE-FTS	MLS
45~55	-5 ~ -20 %	-5 ~ -15%
35~45	< + 5 %	< ±5 %
25~35	< + 5 %	< ±5 %
<25	< + 5 %	< ±5 %

Table 3. Results of coincidence statistics of SMILES HCl (%) compared with ACE-FTS (ver. 2.2) and MLS (ver. 2.2).

Altitude (km)	ACE-FTS	MIPAS
45~55	n.a.	n.a.
35~45	n.a.	n.a.
25~35	0 ~ +10 %	0 ~ +20 %
<25	+5 ~ +10 %	~ 20 %

Table 4. Results of coincidence statistics of SMILES HNO_3 (%) compared with ACE-FTS ver. 2.2 and MIPAS, IMK ver. 40. ACE-FTS and MIPAS HNO_3 are not usable (n.a.) above 35 km.

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