# 5. L2 Data Processing and Product Status

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### 5.0 Outline

- Design and development before launch
  - Were the L2 related activities adequate or not ? Well designed ? Within schedule ? Acceptable processing speed ? Well-prepared for on orbit operation ? Easy to improve ? Well documented and published ?
  - Subjects
    - · Sensitivity study, and design study
    - Forward model: Precision and Accuracy.
    - Retrieval: Setting, A priori
    - Spectroscopy
- L2 Improvement After The Launch
  - Was the L2 system operated and improved appropriately, on subjects, schedule ?
  - Subjects
    - L2: retrieval setting, a priori, retrieval altitude, Tikhonov Regularization
    - · L1B: AOS characteristics, Frequency Calibration, Non-linearity, Pointing knowledge, data flags
    - · Spectroscopy: Spectroscopy review using SMILES data, O3 and O3 isotope laboratory measurements
- Remaining L2 Issue
  - Are the plan for the L2 improvements adequate ?
  - Subjects for future improvements
    - · L1B: Non-linearity
    - · L2 v3.0: a priori modification, Tikhonov regularization to all (as many as possible) species
    - L2 v3.X
      - Baseline fitting for unexpected AOS characteristics
      - Non-Voigt line-shape calculation
    - Spectroscopy: Ganmmaair, n, pressure shift, Non-Voigt line shape.
- Overall
  - Are the L2 related activities performed adequately as the space agency and the science institute ? Are the L2 related scientific results published timely ?

2

# 5. Outline

- 5.1 Design and development before launch
- 5.2 L2 Improvement After The Launch
- 5.3 Remaining L2 Issue
- 5.4 Summary
  - Are the L2 related activities performed adequately as the space agency and the science institute ?
  - Are the L2 related scientific results published timely ?

# 5.1 Design and development before launch

- Were the L2 related activities adequate or not ?
  - Well designed ?
  - Within schedule ? (Schedule management, Budget, Man power/Personel)
  - Acceptable processing speed ? (Algorithm, mathematics, CPU)
  - Well-prepared for on orbit operation ?
  - Easy to improve ?
  - Well documented and published ?
- Subjects
  - Sensitivity study and design study
  - Forward model: Precision and Accuracy.
  - Retrieval: Setting, A priori
  - Spectroscopy

# L2 Algorithm

- Overall requirements described in SMILES Mission Plan (2002)
- Sensitivity study and algorithm design (2006-2009)
- Pre-launch L2 system
- Improvement after the launch
- Remaining Issues

### Characteristics specified in SMILES Mission Plan

- Detail atmospheric and instrument forward model was required.
  - Random noise in spectra, < 0.5K (0.5 s integration)
    - 0.01 K atmospheric forward model precision.
  - Antenna pattern (Mission Plan, 3.2.4.2)
    - Antenna pattern must be considered.
  - Pointing knowledge (relative) (Mission Plan, 3.2.6.2)
    - 0.0015° or 60 m (1sigma), which was found to be performance limiting factor,
  - Sideband Separation (Mission Plan, 3.3.2.2)
  - Acousto-optic Spectrometer, Frequency Characteristics (Mission Plan, 3.3.3.1)
  - Frequency Calibration (Mission Plan 3.3.3.2)
    - as better as 30 kHz

6

### **Mission Plan: Antenna Pattern**



Figure 3.18 Effective antenna response pattern.

### Mission Plan: Image band rejection characteristics (left), and contribution of image band to Band C observation (right)





(c) Image rejection characteristics in LSB. (d) Image rejection characteristics in USB.

Figure 3.31 The effect of the image contributions in Band-C.

Figure 3.28 Coupling coefficient  $K_{ij}$  for signal transmission and image rejection of the SSB filter designed for SMILES. +: Exact theretical calculation for SSB filter; green curves: least-squares fit to the exact calculation; blue curves: simplified model for SSB characteristics of SMILES optics.

### Mission Plan: Characteristics of Acousto-Optics Spectrometer (left) and Spectral Calibration Accuracy (right)



Figure 3.33 Frequency response function of the SMILES/AOS. The typical resolution bandwidth is  $1.35~\mathrm{MHz}.$ 



Figure 3.34 Residuals from the frequency fit with comb generator. 1 Ch. corresponds to approximately  $0.8~\mathrm{MHz}.$ 

9

## Sensitivity Analysis and Algorithm Study

- Sensitivity analysis and Algorithm studies have been conducted JAXA/ ISAS during FY2006-FY2008 (Mar. 2009).
- Forward Model, Inversion, and A Priori have been studied.

#### **Results of Prelaunch Sensitivity Analysis.** 0.01 K forward model precision and Instrument Characteristics affect retrieval are considered as much as possible.



Figure 1.4 Altitude coverage of the JEM/SMILES data estimated from preliminary results of simulation studies assuming 0°N standard profile for each molecular species except for ClO for which the standard profile for polar region is assumed. Refer to Chapter 4 for more details.

SMILES Mission Plan v2.11 (2002)



Takahashi, Ochiai, Suzuki (2010)

11

### A priori accuracy 10° latitude bin, monthly a priori



Fig. 5. Estimations for the influence of priori profiles in O<sub>3</sub> retrieval (in this case, a priori profiles are same as initial profiles). The solid red line is the random error of O<sub>3</sub>. The other lines are additional errors between the true profiles of O<sub>3</sub> and the retrieved profiles of O<sub>5</sub> that are the final results of the iteration process in the cases where the differences between the a priori profiles and true profiles are  $\pm 5\%$ ,  $\pm 10\%$ , and  $\pm 50\%$  (top: mid-latitudes, bottom: tropics). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Takahashi, Suzuki, et al. 2011

# Whole spectra fitting (instead of step-by-step or window approach) is necessary to achieve $1\% O_3$ precision at 20 km. Windowing may introduce >10% error at 15 km or below.



Fig. 2. Simultaneous retrieval of ozone and HOCI. The red (solid) line indicates the retrieval precision in ozone retrieval, the green (dashed) line indicates the incremental error in ozone retrieval without HOCI, and the blue (dotted) line indicates the incremental error in ozone retrieval with HOCI. In all these cases, the true profiles of HOCI are 100% (Right) and 200% (Left) greater than the a priori profile of HOCI. Here, the incremental error is defined as the difference between the true profile and the retrieved profile.

Takahashi, Ochiai, Suzuki (2010)

13

Wind data should be provided for the retrieval. Or, 100 kHz frequency calibration error gives equal to 50 m/s wind velocity error.
10m/s wind velocity error in the stratosphere and 20 kHz frequency calibration error should be achieved. Meteorological data, GEOS-5, is required.



**Fig. 3.** Effect of wind. The red (solid) line indicates the retrieval precision of ozone. The other lines indicate the error due to the difference between the reference profile and the true profile of wind. (The wind velocities for the pink (fine dotted), blue (dotted), and green (dashed) profiles are 50, 10, 5 m/s, respectively. The definition of the incremental error is the same as that in Fig. 2.

Takahashi, Ochiai, Suzuki (2010)

## Elliptical Antenna Pattern requires 2D IFOV integration, 2D IFOV integration with 1° roll precision should be implemented.



Takahashi, Ochiai, Suzuki (2010)



Fig. 3 Two dimensional (Elevation, Azimuth) SMILES antenna pattern.



Fig. 4 One dimensional antenna pattern in elevation axis without antenna motion (dark), and with antenna motion (light).

Suzuki et al., (2011)

15

Antenna pattern including far field affect retrieval. 0-90 km far field is included forward model calculation to achieve 0.01 K forward model precision. But only 5 far field rays must be included to achieve this precision.



Fig. 5 Averaged retrieved profiles (red: moving antenna, blue: fixed antenna), relative difference normalized to a priori of L2 ver. 1.3 O<sub>3</sub> (upper left), temperature (upper right), HCl (lower left) and BrO from SMILES Band A (lower right). 261 observations are averaged in Oct. 12, 2009 at equatorial region N10-S10.

#### Line selection applied to choose 2000-3000 lines per band, 80% of lines are out of band contribution. Weak lines less than 0.01 K are neglected.



Fig. 5. Error due to line selection. The red (solid) line is the retrieval precision of ozone, and the green (dashed) line indicates the incremental error in retrieved ozone due to line selection. The definition of the incremental error is the same as that in Fig. 2.

Takahashi, Ochiai, Suzuki (2010)

17

Forward model: frequency grid: For each AOS spectral bin, 54 (AOS1) and 49 (AOS2) frequency grids must be considered with 0.2 MHz step <±2.4 MHz from AOS center, and 0.4 MHz step at 2.4-8.0 MHz, to achieve 0.01 K radiance precision.

#### Grid pitch of integration of AOS response function

	(AOS1)			(A	OS2)	
Freq. difference from center	Ratio of sensitivity	Freq. step		Freq. difference from center	Ratio of sensitivity	Freq. step
$\cdot 8.0\sim\cdot 2.8$	< 0.02	$0.4~\mathrm{MHz}$	1	$\textbf{-8.0}\sim\textbf{-2.8}$	< 0.02	$0.4 \mathrm{~MHz}$
$\cdot 2.8\sim2.4$		$0.2~\mathrm{MHz}$		$-2.8 \sim 2.4$		$0.2 \; \mathrm{MHz}$
$2.4~\sim~8.0$	< 0.01	$0.4 \mathrm{~MHz}$		$2.4 \sim 6.0$	< 0.01	$0.4 \; \mathrm{MHz}$





図 3.9 AOS 応答関数 (左: AOS1, 右:AOS2)。 横軸はチャンネル中心からの周波数の差。名 兼はチャンネルが異なる。

FY2009 FIP progress report to JAXA (Mar. 2009)

Difference of brightness temperature due to grid correction in integration of AOS response function (integration step: 0.2MHz, integrated range: -40.0 – 40MHz)

~900 frequency grids are carefully selected to achieve <0.001K forward model error by the interpolation at the all 12,000 spectral bins (100 kHz sampling) in the retrieval system.



Takahashi, Ochiai, Suzuki (2010)

# A fast Voigt function algorithm was developed for the L2 forward model



Fig. 2. The five regions in the x-y plane (region 0: Lorentz approximation; region 1: Gauss-Hermite quadrature 2 points; region 2: 4 points; region 3: 5 points; and region 4: 7 points, respectively). The regions 1-4 are originally relevant for Humlicek's approximation of the Voigt profile function. Table 1 Maximum and standard deviation of relative error between Armstrong's and other algorithms for the narrow and the wide range.

Algorithm	Narrow rang	e	Wide range		
	$\epsilon_{\max}$	$\epsilon_{\rm std}$	$\epsilon_{\max}$	$\epsilon_{\rm std}$	
This work	$9.38  imes 10^{-5}$	$1.31 \times 10^{-5}$	$2.52 \times 10^{-5}$	$7.88 \times 10^{-7}$	
Humlicek	$4.88 \times 10^{-3}$	$1.20 \times 10^{-3}$	$8.41 \times 10^{-5}$	$3.09 \times 10^{-6}$	
Hui	$1.05 \times 10^{-3}$	$1.15 \times 10^{-4}$	$1.03 \times 10^{-5}$	$1.80 \times 10^{-7}$	

Table 2

Algorithm	Narrow range ×10 <sup>2</sup> (s)	Wide range ×10 <sup>3</sup> (s)
This work	0.128(3)	0.150(3)
Humlicek	0.627(2)	0.586(4)
Hui	0.136(3)	0.375(2)
Armstrong	3.26(3)	2.435(2)

Imai, Suzuki, Takahashi (2010)

# Spectroscopic studies for SMILES carried out by Prof. Amano et al.



#### O3, pressure broadening. Yamada and Amano (2005)

Line/gas	624.77 GHz		650.17 GHz		
	70 (MHz/Torr)	n	γ <sub>0</sub> (MHz/Torr)	п	
N <sub>2</sub>	3.24 (5)	-0.76 (5)	3.20 (7)	-0.84 (7)	
O2	2.33 (6)	-0.93 (7)	2.41 (6)	-0.70(7)	

Pressure broadening of BrO Yamada et al. (2003)



re with the theoretical Doppler HWHM, the presented here as the HWHM, i.e.  $(\ln 2)^{1/2} T_{co}$ ses with the increase of pressure, and are smaller c calculated for the temperature. The error bars dear one standard deviation estimated by the The horizontal error bars indicate the pressure sequencement

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HCl, freq., pres. broadening, galatry contraction. Morino and Amano (2005).

21

L2 Prelaunch Algorithm satisfied Mission Plan requirements. Even though calculating 10<sup>4</sup> times detailed forward model compared simple model (simulation studies for SMILES), JAXA L2 processing system performed real times basis (L2 processing time is about same of the observation time)

	JAXA (Feb. 2009)
Antenna Pattern	Yes
Image band Rejection	Yes
Acousto-Optics Spectrometer response function	Yes
Out of band lines	Yes
Whole spectrum fitting	Yes

### L2 system



# L2 System CPU Configureation

	Operati on Mgt.	Calc. Node (type A)	Calc. Node (type B)	Backup PC	Web Server	Dev. Support	RAID (type I)	RAID (type II)	Working PC	L2 Switch	UPS
Туре	HP Proliant DL360G5	HP Proliant DL360G5	HP Proliant DL160G6	HP Proliant ML350G5	HP Proliant ML350G5	HP xw8600 CT	Plat'Hom e TrusRAID	Brigad- 3 12FA	HP dc7900	HP ProCurve	APC SmartU PS1500
Model	1U	1U	1U	Tower	Tower	Tower	3U	3U	Desktop	1U	
Number	1	5	3	1	1	1	2	1	3	2	5
CPU	Xeon L5460 3.16GHz	Xeon L5460 3.16GHz	Xeon L5570 2.93GHz	Xeon E5430 2.66GHz	Xeon E5430 2.66GHz	Xeon L5460 3.16GHz			Core2 Duo E7300 2.66GHz		
Core	4	8	8	4	4	8			2		
Memory	4GB	8GB	8GB	4GB	4GB				4GB		
Power	2	2	1	1	2	1	2	2	1	1	1
HDD	72GBx2 (SAS)	72GBx2 (SAS)	160GB (SATA) +4.5TB	72GB (SAS) + 1TB	1TBx2 (SATA) + 1.5TB	500GB + 1TBx3 (SATA)	7TB (SATA)	12TB	250GBx2 (SATA)		
N/W	intra, prv1, 2	prv1, prv2	prv1, prv2	intra	internet	intra, prv1, 2			intra		
OS	RedHat5	Debian 5	Debian 5	Debian 5	Debian 5	Debian 5			Vista		

Other equipments:

19inch rack x 3, Rack mountable console display, Blu-ray drive (for data backup)



# **Inversion model**

#### Optimal Estimation Method + Tikhonov Regularization Method

#### - Observation vector $\mathbf{y} = \mathbf{f}(\mathbf{x}) + \varepsilon$

(x : true,  $\epsilon$  : observation noise , f : Forward Model)

- Deriving the results which minimize  $\gamma^2$ 

 $\chi^{2} = [\mathbf{y} - \mathbf{f}(\mathbf{x})]^{T} \mathbf{S}_{\varepsilon} [\mathbf{y} - \mathbf{f}(\mathbf{x})] + [\mathbf{x} - \mathbf{x}_{a}]^{T} \mathbf{S}_{\varepsilon} [\mathbf{x} - \mathbf{x}_{a}] + \alpha [\mathbf{x} - \mathbf{x}_{a}]^{T} \mathbf{L}^{T} \mathbf{L} [\mathbf{x} - \mathbf{x}_{a}]$ (x<sub>a</sub> : a priori, S<sub>a</sub> : covariance of a priori, S<sub>y</sub> covariance of observation noise,

 $\alpha$ : regulization factor, L: Regulization matrix )

• Non-linear case (Levenberg-Marquardt Method)  $\mathbf{x}_{i+1} = \mathbf{x}_i + \left\{ \mathbf{S}_a^{-1} + \left( \alpha \mathbf{L}^{\mathrm{T}} \mathbf{L} \right)^{-1} + \mathbf{K}_i^{\mathrm{T}} \mathbf{S}_y^{-1} \mathbf{K}_i + \gamma \mathbf{S}_a^{-1} \right\} \left\{ \mathbf{K}_i^{\mathrm{T}} \mathbf{S}_y^{-1} \left[ \mathbf{y} - \mathbf{f}(\mathbf{x}) \right] + \mathbf{S}_a^{-1} \left[ \mathbf{x} - \mathbf{x}_a \right] + \left( \alpha \mathbf{L}^{\mathrm{T}} \mathbf{L} \right)^{-1} \left[ \mathbf{x} - \mathbf{x}_a \right] \right\}$ 

( $K_i$ : Weighting function,  $\gamma$ : Levenberg-Marquardt parameter)

•: exist, •: v1.0, •: v2	Ap	riori	dataset .: v1.0, •: v2
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	Climatolog	3Y			Nearest grid			
	Aura/ MLS <sup>1</sup>	UARS/ MLS <sup>2</sup>	CCSR/NIES CCM <sup>3</sup>	WACCM4 CCM <sup>4</sup>	GEOS-5⁵	WACCM4 CTM <sup>6</sup>	Aura/ MLS <sup>7</sup>	
03			0	$\bigcirc$	0	0	$\bigcirc$	
HCI			0	$\bigcirc$		0		
CIO			$\bigcirc$	$\bigcirc$		$\bigcirc$		
HNO <sub>3</sub>	••		0	0		0		
CH₃CN				$\bigcirc$		•		
HOCI				$\bigcirc$		0		
HO <sub>2</sub>	0			$\bigcirc$		$\bigcirc$		
BrO	0			$\bigcirc$		0		
Temp.	0		$\bigcirc$	$\bigcirc$		$\bigcirc$	•	
Pres.	0		0	$\bigcirc$		0	$\bigcirc$	
Wind			$\bigcirc$	$\bigcirc$		$\bigcirc$		
H₂O	0		$\bigcirc$	$\bigcirc$		$\bigcirc$		

\*1: Monthly average for 2005-2007 by EOS-Aura/MLS v2.2 / \*2: Monthly average for 1992-1994 by UARS/MLS / \*3: Monthly average on the CCMVal-REF2 run for 2001-2010 by CCSR/NIES CCM / \*4: Monthly average for same month by WACCM4 CCM nudged with GEOS-5 / \*5: Near-realtime analyses produced by NASA/GMAO's GEOS-5 DAS included Aura/MLS O3 and Temp /27\*6: CCM Simulations by SD-WACCM nudged with GEOS-5 (not included Aura/MLS) / \*7: Gridded data for same day by EOS-Aura/MLS v2.2





- In addition, band B and C were observed same receivers. So, band A was observed by different receives due to band combinations.
- Number of nominal observed scan was about 1630 per day, howevr, one of retrieved scan was 1400. A few
  percents of scans are not retrieved regularly due to calibration error in brightness temperature. Since the field of
  view of antenna is near the ISS solar paddles, interferences with the paddles caused this error.
- SMILES measured many useful scans which exceed 1200 per day on most days during operation period though irregular data loss like the solar paddle stopping in front of trouble of communication system of ISS/JEM (2010/02/25 – 03/05).

29

# v1.0 (005-06-0024) L2 results example. Kikuchi et al. 2010 $O_3$ and HCI: quite acceptable. Others: need further studies.



Figure 8. Comparison of coincident SMILES and MLS ozone profiles on 12 October 2009 at northern high latitudes: (a) the mean profiles for SMILES (blue) and MLS (red), (b) the differences between the SMILES and MLS profiles in mixing ratio, and (c) the percentage differences.



Figure 9. An example of HCI profiles from SMILES and a comparison with that from ACE-FTS: (a) two profiles from SMILES on 12 October 2009, (1) at 5.1°N and 166.5°E (blue), (2) at 7.7°N and 168.4°E (green), and one profile from ACE on 13 October 2009 at 5.2°N and 170.7°E (red) within 24 hr and a distance of 500 km, (b) the differences between the SMILES and ACE profiles in mixing ratio, and (c) the preeminge differences.



Figure 10. Examples of the retrieved and a priori profiles for (a) BrO and (b) HO<sub>2</sub>. Left: Marks and horizontal bars indicate retrieved values and one standard deviation in red, and those for the a priori profile in blue. Right: S, total error; Sm, massumement error; Sn, smoothing error.

# L2 v1.1 validation trial: O<sub>3</sub>

#### Suzuki et al. 2010 (ISPRS Conference Paper)

MLS

#### ACE-FTS



Figure 2. Example of O<sub>3</sub> 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 5. Statistics of 75  $O_3$  coincidences with 31ACE-FTS (ver.2.2) observations at the 55°N-65°N latitude region.



Figure 3. Example of O<sub>3</sub> 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 6. Statistics of 61  $O_3$  coincidences compared with 284 AURA/MLS (ver.2.2) observations at the  $55^\circ\text{N-}65^\circ\text{N}$  latitude region.



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

**MIPAS (IMK)** 

to Figure 2.

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.



### L2 v1.1 validation trial: HCl Suzuki et al. 2010 (ISPRS Conference Paper)

ACE-FTS



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



Figure 10. Statistics of HCl coincidence comparison with ACE-FTS at the  $55^{\circ}N-65^{\circ}N$  region.

MLS



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



Figure 11. Statistics of HCl coincidence comparison with Aura/MLS at the  $55^\circ\text{N-}65^\circ\text{N}$  region.

### **5.2 L2 Improvements After the Launch**

# • Was the L2 system operated and improved appropriately, on subjects, schedule ?

- Subjects
  - L2: retrieval setting, a priori, retrieval altitude, Tikhonov Regularization
  - L1B: AOS characteristics, Frequency Calibration, Non-linearity, Pointing knowledge, data flags
  - Spectroscopy: Spectroscopy review using SMILES data, O3 and O3 isotope laboratory measurements

# Summary of released v1.X series

- v1.0 (005-06-0024): for retrieval test (2010/01/23 release)
  - Used L2 processing algorithms is designed before launch (Takahashi et al., 2010, Imai et al. 2011).
  - To keep data quality, no-error-flag L1B data were only processed (ratio of processed scan is 55%)
- v1.1 (005-06-0032): for mapping test (2010/04/19 release)
  - To increase processed data, we cope with lack of orbital information from Star Tracker Camera which is one of the reasons of L1B error-flag. (55 -> 85 %)
- v1.2 (005-06-0150): for turned model test (2010/09/15 release)
  - Include turned AOS response model to reduce internal inconsistency.
- v1.3 (006-06-0200): for status flag test (2011/03/02 release)
  - L1B data screening flag updates, etc.

#### Major improvements in v1.X Series: Reducing internal inconsistency

Relative Differences of Temperature (left) and O<sub>3</sub> (right) profile between band A measured AOS1 and band B measured AOS2, single scan



- In V1.1, Temperature, O3 and HCl had 10% difference between band A measured AOS1 and B measured AOS2. in V1.2 suppress them due to response function turning.
- SMILES has 2 acousto-optic spectrometers (AOS) and those response characteristics have been modeled with triple-Gaussian model obtained by ground test data.
  - We included turning factors to response function. It's factor have been adjusted that retrieved temperature agrees with SABER. As the results, differences between band A measured AOS Unit 1 and band B measured AOS Unit 2 became a few percents from 40km up to 60 km.
- In after versoin, we use new response functions obtained by orbit data.

35

# Major improvements (2/2): flag updates

- In v1.2, error flag of FOV interference couldn't reject unusable scans and in v1.3 can due to L1B flag updates.
- There are 2 difference L1B products, L1B and L1B\_rev. L1B is produced from only 1 data, and L1B\_rev is produced from target scan and around 6 successive L0 data in order to reduce the error from receiver drift.
- In L2 processing, L1B\_rev is basically used. However, FOV interference flag in L1B\_rev indicated interference information only for target data, not include for around data.
- New L1B 006 include it. In L2 v1.3, we can reject unusable scans .

Screened data sample (BrO,31km, C, 2010/01/03-24)



# Summary of released v2.X series

- v2.0 (007-08-0300): for non-linear correction test (2011/Oct/03 release)
  - Used New L1B data v007 (including preliminary non-linear correction, ochiai et al. 2012) to improve temperature profiles.
- V2.1 (007-08-0310): L2 algorism update (2012/Jan/12 release)
  - Miner version up to improve only HOCl profiles.
  - It is the first public-release version.

110

- v2.2 (007-09-0400): L2 algorism update (2012 June, Internal release)
  - Update retrieval algorithms and a priori profiles to improve mesospheric profiles.
- v2.3 (007-09-0402): L2 algorism update (2012 Nov., Internal release)
  - Miner version up to improve status flag.
  - used in paper of Stachnick et al. (ACP)
- V2.4 (008-11-0502): L2 algorism update (2013 Jan., Internal release)
  - Update a priori profiles to improvements in mesospheric profiles.
  - used in paper of A. Smith et al. (submitted to JGR)

# L2 v2.0



### **Big impacts of non-linearity correction**



- O<sub>3</sub> and HCl have strong lines in SMILES's bands. These molecules decrease by 5-10 %.
- Since HOCI's lines are located in O3 wing, the profile shape is changed.

39

# **Updates of line parameters**

- We start re-check of line parameters.
- Preliminary updates were included in v2.0 (O<sub>3</sub> line)
   We changed O3 position and pressure broadening parameter, residuals are reduced.



We also changed positions of 18000 lines in band C, and fixed bug about frequency (GHz) grids. It improved 18000 profiles in high altitude.

### V2.0: Correcting Temperature profiles



- SMILES temperature agree with SABER up to 50 km (difference within 1%) , and difference is within 2 % in mesosphere.
  - 2% positive bias in upper stratosphere, and 5% bias in mesosphere is suppressed. They are major issues in v1.3 and it is very good result.
- We can achieve v2.0 objective, to improve temperature profile.
   Next, we check other products..

41

### (preliminary) HCl systematic error analysis

Estimated impact of some systematic uncertainties, like as to *a priori*, line parameter, and retrieval algorithms





- HCl has about 0.2 ppb due to only *a priori* and line parameter's uncertainties.
- In addition, HCl error induced by HCl's  $\gamma_{air}$  error is constant in mesosphere. This shows that SMILES's results might have bias since profile is constant.
- We prepare to estimate another error factor like as radiometric calibration error, other spectroscopy and evaluate HCl systematic error. 42



### **Improvement in HCl products**

- HCl decrease 5% in stratosphere, and 15% in mesosphere. • And We can see one improvement in this version.
- HCl in mesosphere (50-75km) become constant (This feature is suggested by Cl chemistry.) and its value is 3.0 ppb.
  - However, it is necessary to judge this value carefully. (validation results -> Imai et al. (Poster))

# Approach (1/2): for mesosphere

#### Referring more appropriate temperature

- SMILES does not measure O<sub>2</sub> emission lines for temperature retrieval, but used other strong lines, O<sub>3</sub> and HCl.
- However, in mesosphere, since widths of the lines are equal to the frequency resolution of the spectrometers, information of temperature profile is not obtained enough.
- In addition,  $O_3$  and HCl mixing ratios are "variables" and need to be retrieved simultaneously with temperature. It becomes that temperature retrieval is more difficult.



So, in v2.0, we stopped temperature retrieval and referred more appropriate temperature in mesosphere.





10 0 250 0.0 0.5 1.0 Averaging Kernel Temperature (K) In v2.0, GEOS-5 data is used as a priori profile in stratosphere and MLS data is used in mesosphere.

V2.0

Refer a priori

80

70

60

50

40

30

20

- In v2.0, MLS temperature was chosen as *a priori* profiles in mesosphere because of data quantity and quality, and we refer it from 40 km to 90 km.
  - MLS observation covered with SMILES's observation periods, altitude, and latitude. Data quantity are enough to make grid data in 1 day. We can refer same day's data. And data accuracy is < 10 K up to 90 km.
  - Additionally, in order to express migrating tides, Global Scale Wave Model was included.

### Approach (2/2): for upper stratosphere

#### Including gain non-linearity in L1B (Ochiai et al., 2011)

- Gain nonlinearity is scaling parameter of brightness temperature. V1.3 use L1B 006 and this L1B neglected gain nonlinearity. New L1B 007 included this effect measured in pre-lunch system tests.
  - Right figure shows samples of linear and • nonlinear spectra, and difference.
- If neglect gain nonlinearity (v1.3) case), brightness temperature around narrow O3 and HCl lines are overestimated. This may cause positive bias.



114

### V2.1: Minor update version for HOCI



Residual Spectra around the HOCI line band A, AOS2 (N=69) averaged for 1day(2010/04/01), Des, lat S45-S35.





- We prepare minor version up for HOCI. Sample spectrum of HOCI is shown in upper figure.
- HOCl is located near O<sub>3(v1,3)</sub> and <sup>18</sup>OOO. In minor update version, parameters of these lines are changed.
  - Residual spectra is compressed.
  - This version will be released in winter.

### V2.2: improve mesospheric profiles

Retrieved and a priori profile (O3, night) in v2.1 and v2.2 2009/10/17 01:27:56 (N6.48 W18.71 sza 172.64 deg.) 100 00 100 V2.1V2.2 80 80 80 80 Altitude (km) 60 Noisy? 0 60 60 Smooth ! 40 40 40 40 20 20 20 20 A priori A priori Retrieved Retrieved 0 0 0 0 6 9 12 0.0 0.5 6 9 12 0.0 1.0 3 1.0 3 0.5 Ö Averaging Kernel O3 VMR (ppm) Averaging Kernel O3 VMR (ppm)

• In v2.2, new retrieval algorithms, Tikhonov Regularization Method is applied for O3, HCl and HNO3 to smooth profiles and range of retrieval altitude is expanded for O3, HCl and HO2. System return smooth profiles up to 95 km.

## V2.3: Status flag updates

Ratios of useful data (status flag = 0)

	Α	В	С
V2.2	63.0	62.2	29.3
V2.3	94.2	93.9	81.6





- In V2.3, some past conditions like L1B quality and L2 convergence parameter are eased and new conditions are add.
  - standard deviation of residual spectra normalized noise spectra
  - Maximum HCl difference between zonal mean profile and single profile normalized standard deviation (25-80km). Since seasonal and diurnal variations of HCl is smaller than the other smiles products, HCl difference is suitable as a profile quality index.
- Ratios of useful data in each bands are more than 80%, and almost of noisy scan are rejected.

49

### V2.4: mesosphere profile updates

Average of all daytime profiles (SZA < 85°) some instruments(left) and SMILES v2.3, v2.4 (right)



Left panel : Smith et al., 2012, Submitted to JGR, figure 12. "SMILES" is SMILES v2.2.

Upper 80km, SMILES O3 profiles v2.2 is not consistent with other instruments data like SABER, ACE... (Smith et al. 2012).

- In v2.4, some retrieval settings (a priori profiles and error and retrieval altitude range) are changed to reject error due to a priori profile because a priori profile upper 75 km is outside of useful range of MLS O3.
- In v2.4, O3 has sub-peak around 90 km.

#### v2.4: Impact of L1B v008, Frequency Calibration.



L1B v008 (red) is more stable in frequency calibration (±3 kHz) compared to previous L1B (green) (±30 kHz). The smaller frequency jitter should give smaller L2 random error. (Left: AOS1, Right: AOS2)

Frequencies are also changed as much as 100 kHz (left ch900 of AOS1, left). After the L2 v2.0 we have been using O3 frequency different from JPL catalogue, based upon latest laboratory measurement by Dr. Ozeki.

0.0001 0.001 0.1 0.01 10 100 Incremental Error [%]

lid) line indicates the retrieval precision of ozone. The other lines indicate the error due to the difference between the ile of wind. (The wind velocities for the pink (fine dotted), blue (dotted), and green (dashed) profiles are 50, 10, 5 m/s, incremental error is the same as that in Fig. 2.

# v1.0-2.4: Spectroscopy

O<sub>3</sub> and O<sub>3</sub> isotopes: line frequencies have been updated based upon SMILES's own laboratory work after the launch (led by H. Ozeki, Toho U.). If funding will be available, Prof. Ozeki will extend spectroscopy work further.

Other spectroscopic parameters have been reviewed carefully by L2 team and Prof. Ozeki and his colleagues.

Table 5 updated line parameters							
Par	ameters	L2 v1.3	v2.0	Reference			
08							
-	$\gamma_0$ (MHz/hPa)	624371.112	624371.223	Ozeki private communication			
-	$n_{y}$			(preliminary results)			
	,	2.258	2.3078	HITRAN2008			
		0.77	0.78	HITRAN2008			
H85	C1						
-	Line position	625901.603	625901.6584	Colmont et al., 2005			
	(MHz)	625918.756	625918.6975				
		625932.007	625932.0081				
-	$\gamma_0$ (MHz/hPa)	2.57	2.541	MLS Forward model ATBD (v1.0)			
-	$n_{y}$	0.73	0.723	MLS Forward model ATBD (v1.0)			
H <sup>37</sup>	C1						
-	Line position	624964.374	624964.3694	Colmont et al., 2005			
	(MHz)	624977.821	624977.8013				
		624988.334	624988.2821				
-	$\gamma_0$ (MHz/hPa)	2.57	2.541	MLS Forward model ATBD (v1.0)			
-	$n_{y}$	0.73	0.723	MLS Forward model ATBD (v1.0)			
CIC	)						
-	Line position	649445.040	649445.250	Oh and Cohen, 1994			
	(MHz)	649451.170	649451.072				
180	00						
-	Line position	649137.611	649137.132	Ozeki private communication			
	(MHz)	649137.611	649137.132	(preliminary results)			
		649149.603	649152.038				
		649152.601	649152.038				

## **5.3 Future works**

- We plan new version v3.0 in this summer.
  - Update non-linear correction in L1B to reduce difference in receivers.
  - New a priori, SD-WACCM a priori
  - TRM to other noisy molecules is applied and use new a priori data WACCM climatology is used. Profiles retrieved TRM depend on shape of a priori profiles.
  - Non-Voigt line shape.
  - Bias correction of BrO, ClO, HO<sub>2</sub>.
- Future works.
  - Baseline issue caused by the AOS characteristics (over power RF inputs).
  - Gamma-air, temperature exponent (n), pressure shift.
  - any other …

V3.0: Improvements of a priori, SD-WACCM a priori (if necessary and appropriate).



O<sub>3</sub> a priori impacts to O<sub>3</sub>. Takahashi, Suzuki et al. 2011 L2 v2.0: a priori impact to Band C BrO. O3 and BrO have significant impact. (unpublished internal work)

#### V3.0: Tikhonov regularization (TRM) to other species.

Hybrid OEM + TRM technique, i.e. a variation of Tikhonov  $L_0 + L_1$  (similar to MLS ATBD), gave smooth profile, without suffering altitude range or residual increase. It can be applied to all other species. (currently, for O3, HCI, and HNO3) Tikhonov  $L_1$  was used,  $L_1 + L_2$  method may be applied in future.



55

#### V3.0: SMILES L1B vs. L2 Forward calculation shows non-negligible W-shape residual, which should be explained by the non-Voigt line shape.



#### **Galatry and Speed-Dependent Voigt function**

- Voigt function: Gaussian and Lorentzian.
- Galatry function: Narrowing of Doppler width by molecular collision.
- Speed-Dependent Voigt (SD-Voigt)
- Voigt Function
  - Convolution Fourier Transfer of Gauss / Lorentz function V(x) = F(φ(t))

$$\varphi = \exp\left(ix_0t - \gamma t - \frac{\sigma^2 t^2}{2}\right)$$

- Galatry Function
  - Dicke narrowing

$$\varphi = \exp\left(ix_0t - \gamma t - \frac{\sigma^2(1 - \beta t - \exp(-\beta t))}{\beta^2}\right)$$

- Speed-dependent Voigt Function
  - Considering speed-dependence of collision width

$$\varphi = \frac{\exp\left(ix_0t - (\gamma - 1.5\gamma_2 t) - \frac{\sigma^2 t^2}{2(1 + \gamma_2 t)}\right)}{(1 + \gamma_2 t)^{1.5}}$$



#### Galatry and SD-Voigt, impacts to O<sub>3</sub> retrieval are small but different. High altitude (> 50 km) systematic difference from Voigt function may exist.



- Noise at higher altitude can be removed by introducing TRM (from v2.2).
- Impact to daytime ozone:
   Galatry ··· +0.2% (30~40km)、+0.5% (50~80km)
   SD-Voigt ··· -0.2% (20~30km)、+0.5% (50~80km)

#### **Galatry and SD-Voigt: L2 impacts summary**

Product	Band	Ga	alatry	SD	-Voigt
O <sub>3</sub> (day)	А	+0.2%	30~40km	-0.2%	20~30km
$O_3$ (day)	В	-0.2%	10~20km	-0.2%	20~30km
O <sub>3</sub> (day)	А	+0.5%	$50{\sim}80$ km	+0.5%	$50{\sim}80$ km
O <sub>3</sub> (day)	В	+0.5%	50~80km	+0.3%	50~80km
O <sub>3</sub> (night)	А	+0.2%	30~40km	-0.3%	20~30km
O <sub>3</sub> (night)	В	-0.2%	15~25km	-0.3%	20~30km
O <sub>3</sub> (night)	А	+0.5%	50~80km	+0.3%	50~80km
O <sub>3</sub> (night)	В	+0.4%	50~80km	+0.2%	50~80km
HCI	А	-0.3%	15~25km	-0.8%	15~25km
HCI	В	-0.2%	15~20km	-0.4%	15~20km
Temperature	A,B	-0.1K	20~40km	+0.1K	20~40km
HOCI (day)	А	+1%	30~40km	-1%	30~40km
HOCI (night)	А	+2%	30~40km	-3%	30~40km
CH₃CN	А	+3%	10~40km	+6%	10~30km

59

# Galatry and SD-Voigt: Impact to CPU time and the Physics Issue.

- Test L2 code is ready, and increase of CPU time will be negligible.
- The final issue will be which physics we want to use to calculate forward model, Galatry or SD-Voigt ?
  - Need consultation to spectroscopy people.
  - Laboratory measurements to verify, if possible.

V3.0: Bias correction information for BrO, CIO, HO<sub>2</sub>.



# Future: Baseline issue caused by the AOS characteristics (over power RF inputs).

The AOS baseline was found to be distorted by the high RF signal during the lower tangent height atmosphere (i.e. cloud or ground).

The green residual in the figure must be flat at 30, 40, and 50 km, but there are actually not.

This behavior was reproduced exactly after observing the room temperature calibration target and observation of space.



Fig. 6. Averaged spectra and residual spectrum (green: L1B, brown: L2 forward model calculation) of Band C on Oct. 12, 2009 at the equatorial region  $(\pm 5^{\circ})$ , descending orbit, for the tangent height 20 km (upper left), 30 km (lower left), 40 km (upper right) and 50 km (lower right); Number of sample is 37

Suzuki et al. 2012

#### Future: Pressure broadening.

Pressure broadening parameters and their temperature exponent can alter tangent altitude ~500 m easily, which can provide 5-10% O3 and HCl change. Accurate pressure broadening knowledge of O3 isotope will be necessary.



Currently we have been using HITRAN08 for O3 and MLS ATBD for HCl, since it gave agreement of tangent altitude.

Pressure broadening tuning through satellite/ground based validation looks very hard. We expect improved laboratory measurement, but it must be extremely difficult.

63

### **Future: Pressure Shift (1/2)**

From v1.0 to v2.4, we considered pressure shift of O<sub>3</sub> and HCl only. Theoretical pressure shifts have not been applied to other lines. This can be primary reason of large systematic error at lower altitude.



# **Future: Pressure Shift (2/2)**



Figure 3. Broadening and shift measurements of HOCl  $^{\prime}Q_{\sigma}$  branch transitions near 630 GHz.

HOCI, pressure broadening and shift at 630 GHz line. (Drouin 2005).



Fig.3. Effect of Wind. The red (solid) line indicates the retrieval precision of ozone. The other lines indicate the error due to the difference between the reference profile and the true profile of wind. (The wind velocities for the pink (fine dotted), blue (dotted), and green (dashed) profiles are 50, 10, 5 m/s, respectively.

65

# **5.4 Conclusions**

- SMILES L2 prelaunch research and development had been carried out, within schedule under given human resources and budget.
  - Early L2 data showed acceptable results expected from the SMILES specification.
    - Many characteristics of SMILES instrument have been implemented to the L2 forward model.
    - Retrieval scheme, atmospheric forward model, a priori data set, meteorological data, have been prepared adequately for the SMILES launch.
- Extensive updates of L2 system have been conducted since the SMILES operation.
  - Many instrument issues have been pointed out from L2 team.
    - Tangent point knowledge, Frequency calibration, AOS frequency characteristics, Non-linearity correction, flag.
  - Acceptable L2 products v2.1, 2.2, and 2.3 have been released to general public, and several validation works, scientific application have been already submitted or published to journals.
- Plan for v3.0 updates was defined and it can be processed within 3-4 months.
  - a priori updates, TRM to all possible species, Non-Voigt line shape, Bias correction.
- Basic research for future updates (after v3.0) has been conducted.
  - AOS baseline abnormal temporal baseline change.
  - Line frequency, Gamma air, their temperature exponent, and pressure shift.

### L2 related publications

16 papers published (including 3 Spectroscopy, 2 Science), 7-8 other papers have been submitted already. Outline of v2.1 was only published in SPIE, we need detailed algorithm description paper. (There are 10-20 IGARSS, SPIE and ISPRS papers, I could not count.)

- The list only shows 11 papers by core L2 team, not including foreign group or spectroscopy.
- Stachnik, R. A., L. Willán, R. Jarnot, R. Monroe, C. McLinden, S. Kühl, J. Pukite, M. Shiotani, M. Suzuki, Y. Kasai, F. Goutail, J. P. Pommereau, M. Dorf, and K. Pfeilsticker, 2013, "Stratospheric BrO abundance measured by a balloon-borne submillimeterwave radiometer", Atmos. Chem. Phys., 13, 3307-3319, doi:10.5194/ acp-13-3307-2013.
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    - Aura/MLS, UARS/MLS, TIMED/SABER
  - Meteorology/Model :
    - GEOS5, WACCM, CCSR/NIES
- Thank you for your attention!