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Report of SMILES Science Evaluation Panel

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PREFACE

The Superconducting Submillimeter-Wave Limb-Emission Sounder (SMILES) was developed to be 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 by an H - IIB rocket with the H - II Transfer Vehicle (HTV) on 11 September 2009, was attached to the JEM on 25 September, and began atmospheric observations on 12 October 2009 with the aid of a 4 K mechanical cooler and superconducting mixers for submillimeter limb-emission sounding. On the basis of the observed spectra, the data processing has been retrieving vertical profiles for the atmospheric minor constituents in the middle atmosphere, such as O_3 with isotopes, HCl, ClO, HO_2, BrO, and HNO_3. Unfortunately SMILES observations have been suspended since 21 April 2010 owing to the failure of a critical component.

Though the operation time is only for about six months, results from SMILES have demonstrated its high potential to observe atmospheric minor constituents in the middle atmosphere. To evaluate scientific achievements from SMILES we called a panel meeting of the evaluation committee on March 29 and 30, 2013 in Tokyo with attendance of three foreign and four Japanese scientists. The evaluation panel covers the achievement of the SMILES higher-level data processing and related studies on atmospheric chemistry using the data, which were implemented in the Institute of Space and Astronautical Science (ISAS) of JAXA. Based on intensive discussions a report of the SMILES evaluation panel, including recommendations about scientific applications, data improvement, and future mission was concluded at the end of the meeting.

This document summarizes the results of the evaluation panel, and we will continue our efforts for improving the SMILES data products and possible its future mission.

Further information about the SMILES mission including the published data can be found at the following location. http://smiles.tksc.jaxa.jp/index_e.html

September 20, 2013

Masato Shiotani
Leader, SMILES Science Team
Research Institute for Sustainable Humanosphere
Kyoto University

Agenda of the Panel

<u>1st Day (March 28th, 2013)</u>

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(Takayanagi, ISAS/JAXA)
(2) Overview and Scientific Topics
(Shiotani, Kyoto Univ.)
(3) Onboard Operation and Level 1 Data Processing
(Nishibori and Mizobuchi, ISAS/JAXA)
(4) Status of SMILES Project in JAXA
(Sano, ISAS/JAXA)
(5) Level 2 Data Processing System, Retrieval Algorithms & Future Plans
(Suzuki, ISAS/JAXA)
(6) Questions and Discussions

<u>2nd Day (March 29th, 2013)</u>

(1) Discussions with Dr. Newman (via TV conference)

(2) Summary of SMILES instrumental troubles in JAXA
(Sano, ISAS/JAXA)
(3) Preliminary Study for SMILES follow-on
(Suzuki, ISAS/JAXA)
(4) Closed Discussion (Reviewers Only)

(5) Revision of Evauation Report and Wrap-up
(Gille, NCAR)

Evaluation Panel Members

Chair

- Dr. John C. Gille (NCAR)

Members

- Dr. Guy Brasseur (German Climate Service Center)
- Dr. Paul A. Newman (NASA/GSFC)
- Prof. Emeritus Dr. Toshihiro Ogawa (Univ. of Tokyo)
- Prof. Emeritus Dr. Norio Kaifu
(National Astronomical Observatory of Japan)
- Prof. Dr. Hideaki Nakane (Kochi Univ. of Tech.)
- Prof. Dr. Masato Nakamura (ISAS/JAXA)

March 29, 2013
SMILES Science Evaluation Panel

Report of SMILES Science Evaluation Panel

1. Introduction

The Superconducting Submillimeter-Wave Limb-Emission Sounder (SMILES) was designed to be aboard the Japanese Experiment Module (JEM) on the International Space Station (ISS) as a collaborative project between the Japan Aerospace Exploration Agency (JAXA) and the National Institute of Information and Communications Technology (NICT). The mission objectives are: i) Space demonstration of super-conductive mixer and 4-K mechanical cooler for the submillimeter limb-emission sounding, and ii) global observations of atmospheric minor constituents in the stratosphere (O_3, HCl, ClO, HO_2, HOCl, BrO, O_3 isotopes, HNO_3, CH_3CN, etc), contributing to the atmospheric sciences. SMILES was launched on 11 September 2009 by the H-II Transfer Vehicle (HTV), and the atmospheric observations were conducted from 12 October 2009 to 21 April 2010.

2. Scope of the Evaluation

The evaluation panel covers the achievement of the SMILES higher-level data processing (the retrieval of profiles of atmospheric minor constituents from observed brightness temperature spectra in the submillimeter wave region) and related studies on atmospheric chemistry using the data, which were implemented in the Institute of Space and Astronautical Science (ISAS) of JAXA. We have evaluated SMILES outcomes from the point of view of (1) Adequacy of research targets, (2) Research implementation system, (3) Scientific/engineering achievement, and (4) Knock-on effect to the scientific community.

3. Recommendations

Recommendation 1: Scientific Applications

The SMILES instrument was originally designed as an engineering demonstration, with the hope that this new technology would serve the science and provide a unique capability for high-sensitivity atmospheric and astronomical observations. After having established that the instrument was operating satisfactorily and that the quality of the data was high, the science team started to retrieve atmospheric concentrations of key chemical constituents including ozone, chlorine and bromine monoxide, HOCl, HCl, hydroperoxy radicals, etc. The team carefully analyzed the data and was able to derive new information on the chemical and dynamical behavior of chemical species. Among the key findings resulting from this scientific analysis was the quantification of a significant diurnal variation in the ozone concentration as low as 20 km altitude. Since ozone photochemistry is believed to be relatively slow below about 40 km altitude, this diurnal signal must probably be attributed to the occurrence of diurnal tides rather than diurnal changes in photochemical processes. However, this hypothesis needs to be confirmed.

The analysis of the data also showed the capability of the instrument to retrieve the vertical profiles of radical species that are currently not often observed because their measurements are difficult to perform. This is the case, for example, for chlorine and bromine monoxide, which to a large extent are of human origin and provide effective loss mechanisms for stratospheric ozone. The monitoring of such halogenated radicals is key to verifying that the ban in the production of industrially manufactured halocarbons (the Montreal Protocol) is effectively implemented.

A unique aspect of the SMILES observations is the capability to probe the atmosphere from the lower stratosphere to the lower thermosphere and derive continuous profiles over extended altitude ranges. The instrument was able to do its measurements for a period of only 6 months, but this period was long enough to demonstrate the capability of the adopted methodology. During the period of observation, a major stratospheric warming that considerably disturbed the winter extra-tropical stratosphere and a reversal in the tropical zonal circulation associated with the quasi-biennial oscillation took place and provided exciting scientific opportunities for the SMILES team. SMILES measurements are essential to constrain advanced chemical transport models and could be the basis for data assimilation using such models. The scientific benefit of the SMILES mission would be optimal if the observations by this particular instrument could be extended in time and combined with observations of other atmospheric parameters such as the temperature, long-lived tracers and wind components. The measurements of physical and chemical quantities in the lower stratosphere will provide unique information required to do short-term (e.g., seasonal) climate predictions.

The Panel recommends that the analysis of the available SMILES observations be actively continued, and that data be made available to research teams in Japan and abroad. It suggests slightly increasing the funding for the exploitation of the data and to enhancing outreach efforts towards the international research community.

Recommendation 2: Data Improvement

As noted above, SMILES began as a technology demonstration, but has evolved into an instrument of great power and importance for atmospheric science, and an important milestone in Japanese space instrumentation. The science return from SMILES is considerable, but the data are still capable of further improvement, which will further enhance the international recognition it has received. The panel noted that both the L1B and L2 teams had made major improvements in their algorithms, resulting in the present good state of the data. In order to make the future improvements everyone desires, the members of the L1B and L2 teams should work together toward the common objective of improving the data products. Several factors need to be improved in the case of L1B, including further correction for the gain non-linearity. For L2, in addition to reprocessing with the V3 algorithm, further improvements require that improved spectroscopic data be provided.

Therefore, **the Panel recommends that additional funds and human resources be provided to produce improved data processing algorithms, and to apply them in reprocessing the data from the entire mission. In addition, support for acquiring the necessary spectroscopic data should be provided.**

Recommendation 3: Future Mission

The unique nature and high quality of the SMILES data have provided new insights into the chemistry and dynamics of the atmosphere above the tropopause. As noted above, the new characteristics of these data, including the diurnal coverage, observations of rarely or never previously measured radicals and species, and coverage from the lower stratosphere well into the mesosphere and lower thermosphere, have added considerable new information, and are providing strict challenges to models. Unfortunately, the 6-month duration of the SMILES data record, while very useful, is not long enough to see the full range of seasons, the quasi-biennial oscillation, or inter-annual variations. It provides insight into present conditions of temperature and chlorine concentrations, but does not indicate how changes in these conditions may change the chemistry and future dynamics in the atmosphere.

The Panel recommends that JAXA follow up the SMILES experiment with a scientific mission that makes similar (and hopefully expanded) observations of seldom-measured radicals and trace species, showing their diurnal variations, from the upper troposphere into the thermosphere. Ideally this would be coordinated

with other international missions to provide a comprehensive set of high-resolution limb observations.

2013 年 3 月 29 日
SMILES 科学評価委員会

SMILES 科学評価会 報告書 【日本語仮訳】

1. 前書き

超伝導サブミリ波リム放射サウンダ (SMILES) は、国際宇宙ステーション (ISS) 日本実験棟 (JEM) に搭載すべく、JAXA と情報通信研究機構 (NICT) とで共同開発された。ミッション目的は、i) サブミリ波リム放射観測に超伝導ミクサと 4K 級機械式冷凍機を利用する軌道上実証実験と ii) 成層圏大気環境に関連する大気微量成分 (O_3, HCl, ClO, HO_2, HOCl, BrO, O_3 isotopes, HNO_3, CH_3CN, etc) の広域観測の二つである。SMILES は 2009 年 9 月 11 日に宇宙ステーション補給機 (HTV) により打ち上げられ、2009 年 10 月 12 日から 2010 年 4 月 21 日まで大気観測を実施した。

2. 評価の視点

本委員会では、JAXA 宇宙科学研究所 (ISAS) で実施した、SMILES の高次データ処理 (観測したサブミリ波の輝度温度スペクトルから大気微量成分の高度分布を求める計算) とそれらのデータを利用した大気化学の関連研究との達成度を評価するものとする。ここでは、(1) 研究目標の妥当性・(2) 研究実施体制・(3) 科学的・技術的達成度・(4) 科学コミュニティへの波及効果、という観点から成果を評価した。

3. 提言

提言 1: 科学的応用

SMILES の装置は、新しい技術の科学への貢献と高感度な地球大気・天文観測に独特な能力を発揮することを期待して、当初は技術実証用として設計された。この装置が期待通りに稼働し、観測データが高品質であることが確認されたあと、ISAS の解析チームは大気微量成分 (オゾン・ClO, BrO, HOCl, HCl, HO2 など) の量を計算することに着手した。彼らはデータを慎重に解析して、化学成分の化学的・力学的挙動に関する新しい情報を引き出すことができた。科学的な解析に基づく発見の主なものは、高度 20km 付近でのオゾン濃度の著しい日変化を定量的に求めたことである。オゾンの光化学反応は、高度 40km 以下では比較的 遅いものと考えられているので、この日変化は光化学反応の日変化よりもむしろ潮汐変動が原因であると推定できる。しかしながら、この仮定は研究を重ねて確認する必要がある。

データ解析の結果として、SMILES が、従来の観測装置では性能不足のため検出困難であった (化学反応の速い) ラジカル種の高度分布を観測する性能を持つことが示された。例として、人為起源がかなりの割合を占め、成層圏オゾンの破壊メカニズムに大きな影響を与えている ClO や BrO がある。これらのハロゲン化ラジカル種の量をモニタリングすることは、工業用炭素化合物【※フ

ロン等】の生産禁止 (モントリオール議定書) が有効に働いているかどうかを検証するカギとなる。

SMILES 観測の独特な観点としては、下部成層圏から下部熱圏までの大気を探査して、その高度範囲の連続的な大気成分分布を求めていることである。この装置はわずか 6 ヶ月間しか観測実験を行うことができなかったが、SMILES に取り入れられた測定手法の可能性を実証するには十分な期間であったと言える。この観測期間中、北半球の中・高緯度 成層圏に擾乱をもたらした成層圏の大規模な温度上昇と、準二年振動と関連した熱帯域の東西方向の循環の逆転現象が起こっており、ISAS 解析チームにとって科学的な発見をするチャンスをもたらしている。SMILES 観測データは高度な化学輸送モデル計算の制約条件として不可欠であり、そのようなモデルを用いたデータ同化計算の基礎情報ともなる。SMILES ミッションの科学的な利益は、このような装置による観測が、今後 引きつづき、温度や長寿命の微量成分【※二酸化炭素など】や風速の観測と併せて実現されれば、最大限に引き出される。下部成層圏の物理的・化学的な量を測定は、短期の気候予測 (例えば季節変動など) に必要な独自の情報である。

本委員会は、SMILES で得られた観測データの解析を今後も積極的に継続することと、得られたデータを日本国内および海外の研究チームが利用しやすいよう整備することを勧告する。データの利用促進や国際的な研究団体への働きかけのための予算をもう少し手厚くすることも提案する。

提言 2: データの改良

前述のとおり、SMILES は技術実証として始まっているが、大気科学として強力かつ重要な観測装置へと発展しており、日本の宇宙機器の重要なマイルストーンになったと言える。SMILES 観測によって得られた科学的成果は注目に値するものであるが、観測データはさらなる改良を加える余地があり、国際的な評価もますます高まると考えられる。本委員会は、L1B 解析チームと L2 解析チームとがそれぞれのアルゴリズムを大きく改良しており、それにより現在の精度良いデータが存在する、ということを認める。期待される将来の更なる改良を実現するために、L1B 解析チームと L2 解析チームは、データプロダクトをより高精度のものにするという共通の目的に向かって、一体となって取り組むべきである。L1B データについては、ゲインの非線形性を含む、いくつかの改善すべき問題点がある。L2 データについては、【※評価時点で開発途中であった】バージョン 3 アルゴリズムによるデータの再処理に加えて、更なる改良を施すために高度な分光実験データを取得する必要がある。

そのため、**本委員会は、予算とマンパワーとを追加して、データ処理アルゴリズムの改良を行い、そのアルゴリズムを用いた全期間のデータ再処理を行うことを勧告する。加えて、必要な分光実験データを取得するための支援も行うべきと主張する。**

提言 3: 将来ミッション

SMILES データの独自の性質と高品質とにより、成層圏以高の大気の化学と力学に関する新しい知見がいくつも得られた。前述のとおり、SMILES データの新しい特色である、一日の様々な時間帯を観測したこと、これまで観測例が全く無いかほとんど無かったラジカル種や化学種を観測したこと、そして下部成層圏から中間圏・熱圏に至る広い高度範囲を観測対象としたこと、これらは新しい情報をもたらすとともに、モデル計算に厳しい制約条件を提示した。SMILES データの 6 ヶ月間という期間は、有益ではあるが、季節変動・準二年振動・経年変化を扱うには残念ながら不足している。SMILES データは、温度と塩素量との現状を理解するのには役立っているが、現在の条件において、大気の化学的・力学的状況が将来的にどのように変化していくかを示すことはできない。

本委員会は、JAXA に対して、SMILES 観測実験の続編となるような、SMILES と同等の (または更に拡大した) 観測困難な化学種の、日変化を示せるような、上部対流圏から熱圏に至る高度範囲の観測を行える科学的ミッションを実施することを勧告する。このようなミッションは、高精度リム観測の総合的な観測システムを構成するために他の国際的ミッションと連携して実施できれば、理想的である。

以上

SMILES Science Evaluation Panel

(Summary)

Date: 28-29 March 2013

Venue: Tokyo Office of Kyoto University, Tokyo

DAY ONE

Introduction

Dr. Takuki Sano opened the meeting, explaining the distributed meeting materials and schedule.

Welcome Remarks / Scope of Evaluation Panel

Dr. Masahiro Takayanagi was asked to offer welcoming remarks. He also presented on the scope of the Evaluation Panel.

Discussion

Dr. Norio Kaifu: Who does the Panel reported to?

Dr. Takayanagi: The Science Steering Committee of ISAS.

Dr. Kaifu: Should the panel's report be limited to science? SMILES started as an engineering program. How have the engineering results been evaluated?

Dr. Takayanagi: A separate panel has already evaluated the engineering.

Dr. Kaifu: I would like to view the results of that panel. Will we produce a draft report tomorrow?

Dr. John C. Gille: That is the plan.

Overview of SMILES Mission and Scientific Outcomes

Dr. Masato Shiotani gave a presentation on the scientific outcomes of SMILES.

Onboard Operation and Level 1 Data Processing

A presentation was given by Dr. Toshiyuki Nishibori and Dr. Mizobuchi on the L1 data from SMILES.

Discussion

Dr. Kaifu: You noted that local oscillator broke. Do you know why?

Dr. Nishibori: It was due to the low reliability of the diodes used. Normally, spacecraft are using high reliability diodes, but we used a commercial part with low reliability because we needed a unique design given the lack of space.

Dr. Gille: Even with the correction to non-linearity, there are still some deviations. Can you improve that?

Dr. Mizobuchi: We are still studying that.

Dr. Gille: In the spectrum comparison, it looks like there are significant changes in the continuum – at 625 GHz, for instance.

Dr. Mizobuchi: Depending on the place, we changed the altitude. That is the difference. The lines just show sample positions.

Status of SMILES Project in JAXA – Schedule, Resources and Implementation

Dr. Sano gave a brief presentation on the status of the project in JAXA.

Discussion

Dr. Gille: Level 1B processing seems to end in 2012. Is it possible to improve L1B results?

Dr. Sano: We are thinking of extended studies combining L1B and L2 improvements.

Dr. Kaifu: You said you had many problems related to the lack of schedule management. Were those expected or unexpected?

Dr. Sano: We would implement a solution, and that would cause another problem to occur. We could not always foresee the results of what we did.

Dr. Guy Brasseur: We heard that you made a call for projects. The research team you presented in relation to that seemed international. Do they come to Japan to work with you? Do they get money from you?

Dr. Makoto Suzuki, ISAS/JAXA: Only 10 came to the workshop held in Japan in 2010. The researchers must find their own funding.

Dr. Hideaki Nakane: You presented self-ratings. Should the panel evaluate the self-ratings?

Dr. Sano: The evaluation results are up to the panel members.

Dr. Suzuki: You should evaluate Dr. Sano's work as well. Please evaluate whether data retrieval and evaluation has been properly done.

Dr. Kaifu: I strongly feel that it is difficult to evaluate only science without considering engineering or such matters as how JAXA has supported this project. I want to know about the other circumstances of SMILES.

Dr. Gille: Will we be able to see the engineering evaluation?

Dr. Takayanagi: Of course.

Dr. Gille: Can you talk about the effort rates of each person involved in SMILES.

Dr. Suzuki: I am part-time on this project.

Dr. Kaifu: The organization for the science was poor at the start. It improved over time. I think we need to consider this.

Dr. Brasseur: This is probably because the instrument was regarded as an engineering project, and the science was only considered later.

Level 2 Data Processing System, Retrieval Algorithms & Future Plans

Dr. Suzuki presented.

Discussion

Dr. Masato Nakamura: How much budget and manpower is needed for the continuation of the project?

Dr. Suzuki: I cannot say about budget. We now have two post docs, but starting from April, we will have none. This is an issue.

Questions and Discussions

Dr. Gille: The standard of work is very high. I want to discuss the overview and science topics mainly. Do the panel members have any comments?

Dr. Brasseur: I was impressed by the investigation. When I look at existing spacecraft worldwide, SMILES is certainly very much at the top in terms of looking at the diurnal variations of a number of compounds. I would like to know about the mining of data over the months. What is the view you have on taking full advantage of these data to do frontier science? How are the projects organized? How can you bring new talent into the analysis of data? What is planned?

Dr. Shiotani: Because of the limitation in terms of time, it is difficult to do frontier science. We don't have constant band results. In that sense, a variation study would be appropriate for SMILES. It is difficult to do a time series analysis.

Dr. Kaifu: There are other, similar satellites such as MLS. Besides the calibration of instruments, what new achievements have been made for this kind of data processing?

Dr. Suzuki: For data processing, we are among the best. Retrieval systems are similar to those used by other groups.

Dr. Shiotani: Many researchers recognize the importance of non-linearity, but until SMILES, no one had done it before.

Dr. Suzuki: In the past, similar kind of non-linearity correction was done in detail for ADEOS/IMG. I also proposed it to GOSAT, but they did not like it.

Dr. Nakamura: It is a pity that the observations were only done halfway. What are your future plans for SMILES?

Dr. Suzuki: I am considering how we should make a proposal about that. So far, only a few researchers are interested. Satellite projects are huge commitments. I believe we should measure wind velocity and temperature. We are talking to NOAA about this. If we decide to use their instrument in the Japanese station, they can deliver us such data.

Dr. Shiotani: The budget in Japan is such that we cannot measure temperature. We now realize that we need a temperature sensor. If we create SMILES II, we would like to include that.

Dr. Nakamura: The mission budget for small satellites is about US$20 million.

Dr. Suzuki: That is about half of what we would require for SMILES II.

Dr. Kaifu: I would like to get a better understanding of the scientific results of this project. What sort of impact do you think SMILES has had on atmospheric science?

Dr. Shiotani: The most important one is the information about diurnal variations in the atmosphere. Now we can clearly see the diurnal cycle. We cannot clearly see its importance, but we can clearly see it exists.

Dr. Brasseur: The vertical range of the reading is unique as well, discovering even a diurnal cycle at such low altitudes. Contrasting the way the cycle changes as we move up is very important. I also think the satellite is optimal for studying a variety of chemistry interactions in the atmosphere. There is a real vertical profile here. The weakness of the data is that the timeframe is too short.

Dr. Gille: I agree. I thought that having a 4 K cooler was a real engineering feat. I believe the mixer technology was excellent as well. It produced data with lower noise than MLS. We cannot take full advantage of the low noise without understanding any systematic effects though.

Dr. Kaifu: I didn't see much about CH3CN. It is a signal of biomass burning that reaches the stratosphere.

Dr. Suzuki: The profile of that looks alright, but we are not ready to present that data. We are still trying to retrieve it.

Dr. Nakane: I was impressed with the spectrum and the professional work of the SMILES team. They have created important information from the L1 product. I think the collaboration of L1 and L2 is important. I feel that they have not fully demonstrated the full potential of the data. The future prediction of the ozone layer presented had large scatter. I am not sure that the ClO data, BrO data, and so on can help to reduce the scatter in this prediction. The chemistry and dynamics of the stratosphere are not fully understood. If the full potential of SMILES data was used, could the scatter be reduced?

Dr. Shiotani: The future prediction heavily relies on the chlorine scenario. The chlorine amount is critical, so the SMILES data affects the prediction that way.

Dr. Gille: The diurnal prediction could also point out how certain data need to be changed. Do you have a list of things that could be done in the future with this data, or perhaps if improvements are made?

Dr. Shiotani: Horizontal BrO is something we are interested in. We should demonstrate SMILES' ability with ozone, ClO, and other species that people are familiar with. After that, people may be more ready to believe our results in other areas.

Dr. Suzuki: We can theoretically calculate the day and night HO_2 at the same location in the day and night on the same day. One suggestion is that we look at ClO+HO2 reactions.

Dr. Shiotani: Additionally, We see very clear evidence of the diurnal cycle in HOCl, and that is a topic we are interested in investigating.

Dr. Brasseur: You are using WACCM, but you don't have it in house. Wouldn't it make sense to use it here?

Dr. Suzuki: It could be run, but we have no manpower for that.

Dr. Brasseur: If you really want a good interpretation, you need to have that kind of models. The other point I wanted to ask about was retrieval – are you in contact with the MLS team or other international teams?
Dr. Suzuki: There is a joint-international team in NICT, and we occasionally discuss with their members about our work. Members of the MLS team have joined our meetings before and given us comments.

Noting the time, Dr. Gille brought the day's discussion to a close.

DAY TWO

Open Discussion

The day's discussion was joined by Dr. Paul A. Newman via Skype. Dr. Gille offered to first review the previous day's discussion. After that review, Dr. Newman was invited to pose questions.

Dr. Newman: SMILES is still up on the ISS?

Dr. Shiotani: Yes. JAXA has been investigating the possibility of replacing or repairing SMILES, but that is almost impossible. It will be deorbited.

Dr. Newman: It looks like great data. It would be nice to have a SMILES II orbiting for a few years. That is my main thought.

Dr. Brasseur: What is the longest period of operation that one could expect?

Dr. Suzuki: Two years is reasonable due to lifetime of cryocooler, but my dream is three years. It is costly.

Dr. Brasseur: Originally, this was a technological mission to see if the 4 K cooler could work. They only realized later that the science was good.

Dr. Newman: I recognized that the instrument was a great achievement.

Dr. Brasseur: Diurnal variation was observed on species very low down in the stratosphere.

Dr. Newman: After looking at the ozone diurnal cycle results, that was one of the things that I noticed immediately.

Dr. Gille: I would urge that more effort be put toward improving the L1B in order to allow better L2 results. I also suggest we recommend that they continue interaction between L1B and L2.

Dr. Brasseur: There are still some uncertainties about spectral parameters. It would be useful to have better spectral data.

Dr. Suzuki: It is our biggest limitation right now. We are working with universities in Japan and France to calculate spectral data. Many groups have been measuring pressure parameters, but each shows different results. We need to first think about the best method for measurements. We are discussing this. Our frequency standard in the lab has improved.

Dr. Newman: I would like to offer my comments. I think the data looks great. The low altitude spectra are beautiful. I was impressed at the progression of the algorithms. It is critical to have a feedback loop between the improvement of data and science that is needed. I think that SMILES could become a fundamental instrument for stratospheric science. I like the idea of regular processing. Was the research target of SMILES appropriate? I think it was very appropriate. The minimum objectives were good. The research implementation was done well also. The minimum goals were met, and for a six-month period, they did well. There was major warming, there was the fall to spring northern hemisphere transition, and a number of other research topics covered. It was a good six months. I like the research funding. I also like the connections to cooperating institutions like MLS. It may be worthwhile to reach out to the SAGE team. There are lessons SMILES could take from TOMS. The first lesson is that the TOMS people gave out free CDs with all of their data, and a few months after that, the number of publications jumped. The second thing they did was they put the data out for free on the internet. That also created an upward spike in the number of papers being written. Was implementation system of SMILES research properly established? The more people who look at your data, the more problems people find, and the more you can do to correct your data. The seeding of research funding sets this in motion. We can see the number of publications starting to increase. I recommend a little more research funding and outreach to the general community. Did SMILES achieve its research target? The minimum targets were more than achieved. It is unfortunate that only 191 days of measurements were done, but things are working out. I think the results will have impact, especially in relation to the diurnal cycle. The extra HCl data that is between the low values from HALOE and higher values from other instruments will have impact. It would be good to have several years of measurement for HCl. I believe that there is room for improvement on retrieval. I also believe that we need to have continuous improvement and the achievement of the maximum quality from the data set. Has there been significant collaborative effect in the scientific community? I guess that this is true. The publication of the data and outreach to the community will begin to make the data more known and I think we will naturally see more collaboration.

Dr. Brasseur: Do you think the international community knows that SMILES exists? Is there a need for more presence?

Dr. Newman: I think it is known at a certain level. They knew it flew. That is different from seeing the data and papers published on it. I think that if people cannot get data easily, they will quickly abandon efforts to use it. An outreach effort is still required.

Dr. Gille: Has the SPARC Data Initiative helped to get it visibility?

Dr. Newman: I do not have a real opinion on that.

Dr. Brasseur: So the recommendation is to be very present at international conferences and so on, to promote the data?

Dr. Newman: I know people are aware of the data, but I do not know how people are using it. It may help to talk to people. Please keep me informed about SMILES II, I will be a real advocate.

Having finished his comments, Dr. Newman said goodbye to the meeting and signed off. Dr. Sano then presented a summary of SMILES instrumental trouble.

Dr. Gille: Did you ever consider making a high reliability Gunn diode?

Dr. Suzuki: We expected the diode used to last for around seven years, but it only lasted six months.

Dr. Kaifu: It is well-known that Gunn diodes can break. It is important to have a redundant design.

Why didn't you make such a design?

Dr. Suzuki: There was a shortage of time and money.

Dr. Sano: NICT has said that they inspected more than ten Gunn diodes and chose the best one, but it still broke.

Following Dr. Sano's presentation, Dr. Suzuki presented on a proposal to use a 400 kg Japanese small science satellite for stratosphere-mesosphere science.

Dr. Brasseur: What is the weight of SMILES?

Dr. Suzuki: Including the frame, it is 500 kg, but inside it is probably about 200 kg.

Dr. Kaifu: Why don't you make the SMILES II proposal worldwide?

Dr. Suzuki: There is no money for that. Today we have half the SMILES committee. There is another group in NICT proposing a room temperature technology instrument, but they do not have interest in a 4 K instrument.

Dr. Gille: I think there was a question of how much the non-linearity could be improved. I am not sure how directly that affects the retrievals.

Dr. Shiotani: We understand now that better results could be achieved with our experimental non-linearity correction. We need to study this further. We are still doing data processing.

Dr. Gille: What particular results are improved by better non-linearity?

Dr. Suzuki: We have no clear idea. The L2 group can probably search for the best combination of non-linear corrections by checking our retrievals.

Dr. Kaifu: There was no formal review of the engineering part of SMILES. I have only seen fact reports and analysis.

Dr. Suzuki: SMILES instrument performance was carefully reviewed during the Nominal Operation Review.

Dr. Kaifu: Was that held already? Did they create a report?

Dr. Sano: It was done in October 2010. They wrote a detailed report in Japanese.

Dr. Suzuki: My feeling is that the report states that the engineering was just so-so.

Dr. Gille: We could say for this report that the instrument was an important part of the experiment, and an outstanding technical achievement for the period that it operated in. We might also say that we now know more about the data, and we recommend stronger effort to improve the L1B. That should go along with the work on L2 and for version 3.0.

Dr. Kaifu: Will we mention the future possibilities of SMILES?

Dr. Gille: As a member of the ISS Steering Committee, do you think it would be appropriate for us to talk about?

Dr. Kaifu: If you feel it is very important, new technology that opens the scope of atmospheric science, than they should consider the next step.

Dr. Brasseur: SMILES started with a prototype with the hope that it would be important for science. That has been demonstrated. The period was only for six months, and that was a limitation. The program produced some unique results, but it also did not produce others because the instrumentation was not appropriate. It could be very promising when combined with other instruments. It could really become the backbone of a large international space experiment. With that kind of program, you could probably go further down too, and that would be very important.

Dr. Gille: I worry about endorsing something too specific.

Dr. Brasseur: I do not want to be specific. But it could compliment a broader future program.

Dr. Kaifu: For JAXA, this was an engineering test to create new science. It is important to recommend what they should do from now.

Dr. Nakamura: ISAS asked Dr. Shiotani to be a visiting professor. We want him to propose a small satellite mission. We have extended his duties for this reason. There is a high chance of this becoming a small satellite if he proposes it.

Dr. Gille: The unique aspects of SMILES, such as the additional radicals, would be beneficial for other missions.

Dr. Brasseur: For the report, I think it is good to have a limited number of recommendations. In the end, people read only the recommendations. They are more powerful if we only list two or three.

Dr. Gille: I will start with three: 1) Continue to exploit the data that we have now. They are good and should get a lot of attention. 2) Improve the data beyond where they are now by a) improving the L1B, especially the non-linearity, and b) extending the L2. 3) Consider the future flight of an instrument or instruments that would consider some of these measurements, especially the diurnal variation, seldom measured species and radicals, and large vertical range. This should happen as part of a worldwide program, as a science mission.

Dr. Brasseur: It is not a recommendation, but I think we need to write very clearly that the approach used started with a technology project, demonstrated that it was compelling to do some science investigation, and the program has been very successful in that regard. The time has come now to apply the technology. In other words, mission accomplished.

Dr. Gille: I think we should avoid endorsing a particular technology.

Dr. Brasseur: Yes, but we should say that the approach taken has led to success. That is the basis for the third recommendation about future missions.

Dr. Toshihiro Ogawa: Concerning that recommendation, in the ISS discussions, there several research fields fighting to continue their work. I feel that stratospheric science is rather mature. Recommending simple continuation is, I feel, a weak recommendation. We should emphasize new science.

Dr. Brasseur: The question is, is there a scientific need to continue this work? You could say that other work is more important. We need to address this issue.

Dr. Gille: We did not see a complete QBO. We have little information on diurnal variability. There are reasons to continue.

Dr. Brasseur: In the climate community, the focus is on the next ten years. Is there predictability to climate like there is predictability to weather? One key to understanding this is the stratosphere. In particular, an understanding of the lower stratosphere over the long-term is crucial.

Dr. Gille: The stratosphere is changing. We think we understand diurnal variation now, but will that work ten years from now under various conditions?

Dr. Brasseur: This experiment is not strong on long-term trends. However, after this, others will make measurements, and a detailed analysis of two or three years will help us understand long-term trends.

Dr. Suzuki: The upper mesosphere is also a new challenge for chemistry.

Dr. Brasseur: Would there be a way to see the polar regions in the future?

Dr. Suzuki: We can either choose to see most of the northern hemisphere or have two fields of view.

Dr. Brasseur: How long should the report be?

Dr. Shiotani: The report will be sent to the Science Steering Committee in ISAS.

Dr. Suzuki: The report will be sent in May, and we should send it about two weeks before that meeting. You are not required to finish it today.

Dr. Nakamura: It should be maybe two or three pages.

Closed Discussion

Following lunch, the Dr. Gille and Dr. Brasseur prepared a draft report. It was shown to the entire group for discussion upon its completion.

Revision of Evaluation Report and Wrap-up

Dr. Gille: We covered the background, scope of evaluation, and recommendations related to science. We recommend that the measurements continue, touch upon how highly successful the instrument was, and call for additional funds and resources for an improved L1B algorithm. We also recommend that L2 data be processed with the version 3.0 algorithm. In the future, we recommend that JAXA follow up the SMILES experiment with a mission making similar observations of seldom measured radicals and species.

Dr. Brasseur: In recommendation 1, I note that the instrument was originally designed as an engineering prototype. I also mention key findings related to a significant diurnal variation in the ozone concentration as low as 20 km. The analysis of the data showed the capability of the instrument to retrieve vertical profiles of radical species that are not often observed. A unique aspect of SMILES is the capability to probe from the lower stratosphere to the lower thermosphere. The experiment demonstrated the capability of its adopted methodology. I recommend the combination of SMILES data with other parameters such as temperature, long-lived tracers and wind components. I recommend the active continuation of SMILES, with the addition of resources from Japan and abroad.

Dr. Gille: It is very nice. If there is anything inaccurate, we should fix it.

The meeting discussed changes to the wording of Dr. Brasseur's section.

Dr. Brasseur: Do you want to add HOCl or HCl to the list of chemical constituents monitored?

Dr. Suzuki: Yes.

Dr. Brasseur: Were you able to look as low as 20 km? Or was it 25 km?

Dr. Suzuki: 20 km is alright.

Dr. Gille: The important thing is whether or not everyone is happy with the recommendation.

Dr. Suzuki: My concern is that there is no mention of the importance of spectroscopy.

Dr. Gille: So we will need to add something, I suppose in relation to L2. In recommendation 2, I noted that we all felt SMILES was a success in the period it operated in and that the work to produce three upgraded versions was very good. I mentioned that the experiment met pre-launch requirements. Is that true?

Dr. Suzuki: Yes.

Dr. Shiotani: This is really what we need for panel members to say, but is it really comfortable for environmental people? I think mutual collaboration is very important. Perhaps recommendation 2 and 3 should be combined.

Dr. Gille: If you think it would be better to link the L1B and the L2, I can rewrite the recommendation to mention this.

Dr. Shiotani: We do not want to divide responsibility. Both L1B and L2 processing are very important.

Dr. Gille: So we will recommend the continuous improvement of the data, including collaboration between the two groups.

Dr. Nakane: The feedback cycle between the two has been very fruitful.

Dr. Brasseur: We should say that there should be further collaboration.

Dr. Shiotani: There is still some division between the L1B and L2 processing teams. It is an unfortunate condition.

Dr. Gille: I would hope that the institutional barriers are not great and that human interaction can make it work.

Dr. Nakane: Collaboration will be necessary if there is to be an extension.

Dr. Gille: The panel encourages the members of the L1B and L2 teams to continue to improve their communications such that seamless data processing can occur. Would something like that be alright?

Dr. Shiotani: Yes.

Dr. Gille: In terms of a future vision, I noted that SMILES provided unique insights and has new information on rarely or never-before measured radicals. I also commented that the six-month duration was not long enough to see the full range of seasons. I recommend that JAXA follow up the experiment with a mission to make similar measurements coordinated with other international missions to provide a comprehensive set of high resolution limb observations.

Dr. Kaifu: I think it is convincing.

Dr. Gille called for a coffee break so that he could merge recommendations 2 and 3. Afterwards, the meeting continued discussion on the recommendations.

Dr. Gille: I combined recommendations 2 and 3. I talk about SMILES as an instrument of great power and importance, calling for additional funds and human resources to produce improved data processing algorithms and then apply them to reprocessing.

Dr. Brasseur: We should add a sentence about spectroscopy.

Dr. Gille: We can propose that for L2 improved spectroscopic parameters are needed.

Dr. Shiotani: We recognize spectroscopic parameters and gain non-linearity as very important, but these are just examples of important issues. The recommendation may be too specific.

Dr. Gille: We use the term feedback, and that tends to be from L2 to L1. I do not want to imply that.

Dr. Shiotani: Perhaps it could be phrased to say something like “one example of an important improvement is the consideration of gain-linearity.”

Dr. Brasseur: This recommendation should be more direct.

Dr. Gille: The last sentence before the recommendation says that we need it and the recommendation says that resources should be provided for it.

Dr. Suzuki: Professor Hiroyuki Ozeki is one Japanese scientist that could help us with spectroscopy. We should encourage that. From the viewpoint of ISAS, the recommendation is alright, but others may feel it is too strong.

Dr. Kaifu: I do not know the background of organizational issues. From a scientific viewpoint of the science, this is alright.

Dr. Gille: Even if someone from JAXA should see this, we are saying that the instrument has done well and there is a chance to show it is even better. I think it is alright.

Dr. Kaifu: It may be too strong to say that L1B and L2 should work as a single team.

Dr. Suzuki: That is meant to be a strong request that Dr. Nishibori work more closely with us.

Dr. Kaifu: It is obvious that this is a single mission and both groups should work together. Probably we should say that the panel recognizes there is the existence of a problem related to collaboration.

Dr. Suzuki: It would be nice to move Dr. Nishibori to ISAS.

Dr. Kaifu: We cannot touch such matters. Just write that the members of the teams should work together toward the common objective.

Dr. Nakane: Why has there not been enough cooperation so far?

Dr. Suzuki: One reason is that we are geographically separated by 100 km. My feeling is that Dr. Nishibori should physically come to ISAS more often. In addition, the budget is divided between two teams. Those are the issues.

Dr. Nakane: There is collaboration, it just needs to be enhanced.

Dr. Gille: Can't you work by e-mail, telephone, and Skype? It should not be such an impediment.

Dr. Nakamura: These are all internal issues.

Dr. Kaifu: I think we should just touch upon the importance of coordinated work and leave it at that. We must avoid negative comments.

Dr. Nakane: If the wording is too weak, I get the impression that we are accusing them of not working together until now.

The wording of recommendation 2 was reworked and approved. The meeting then discussed text style changes to the document.

Dr. Gille: Anything else?

Dr. Shiotani: I would like to add a sentence mentioning the relation to modeling activities.

Dr. Brasseur: To recommendation 1, we will add that SMILES measurements should be used to constrain advanced chemical transport models.

Dr. Kaifu: That is more of a recommendation to the entire scientific community than to ISAS.

Dr. Gille: Anything else?

Dr. Kaifu: Do you need the report immediately? I would like to send the draft to Dr. Newman. Let's send it to everyone, and we can finalize it over a span of three weeks.

Dr. Gille: That will give us time to communicate.

Closing Remarks

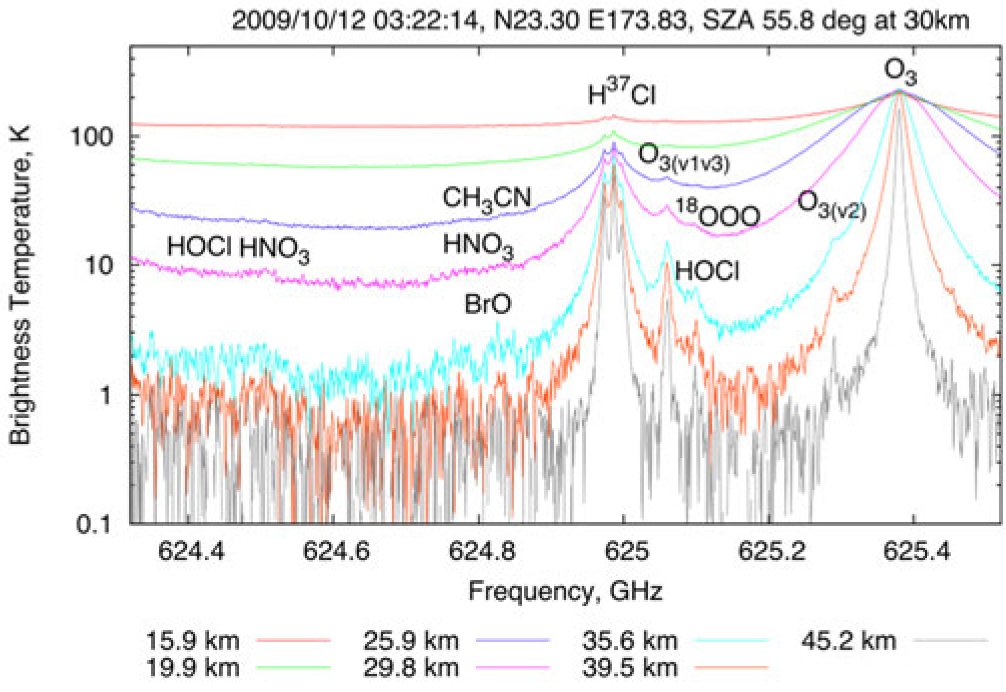
Seeing that there was agreement about the report and no other points to discuss, Dr. Gille closed the meeting.

Presentation Materials

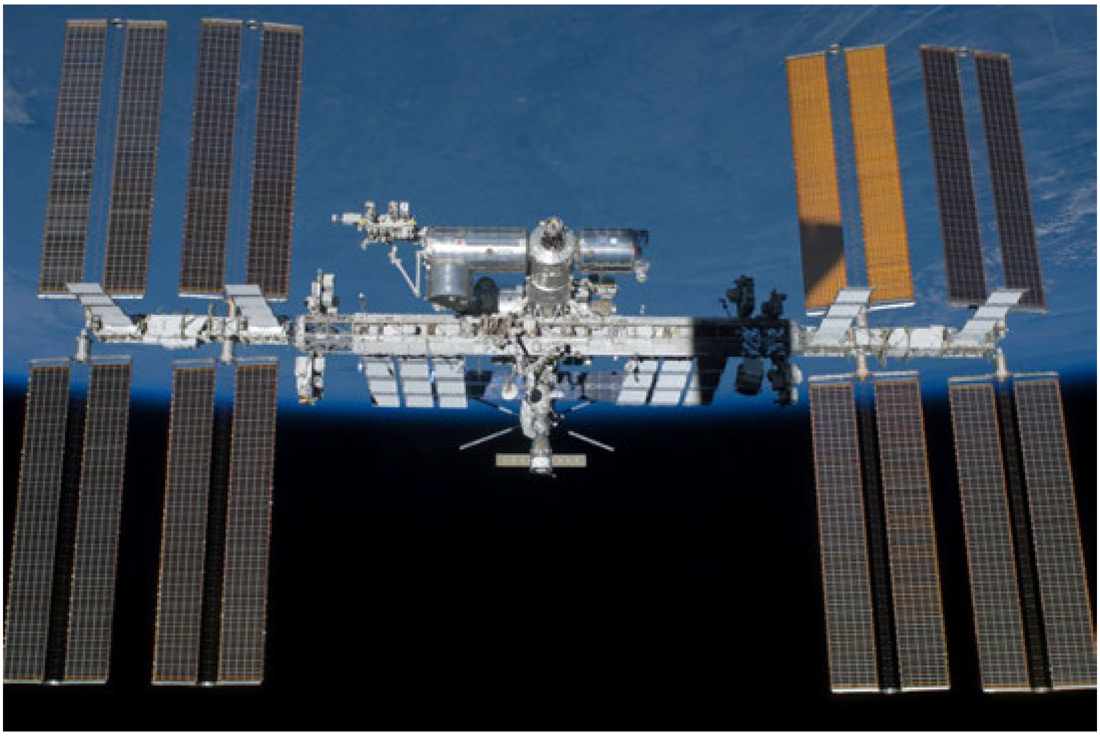
Scope of Evaluation with the Panel

Masahiro TAKANAYANAGI
Director of ISS Science Project Office,
ISAS / JAXA

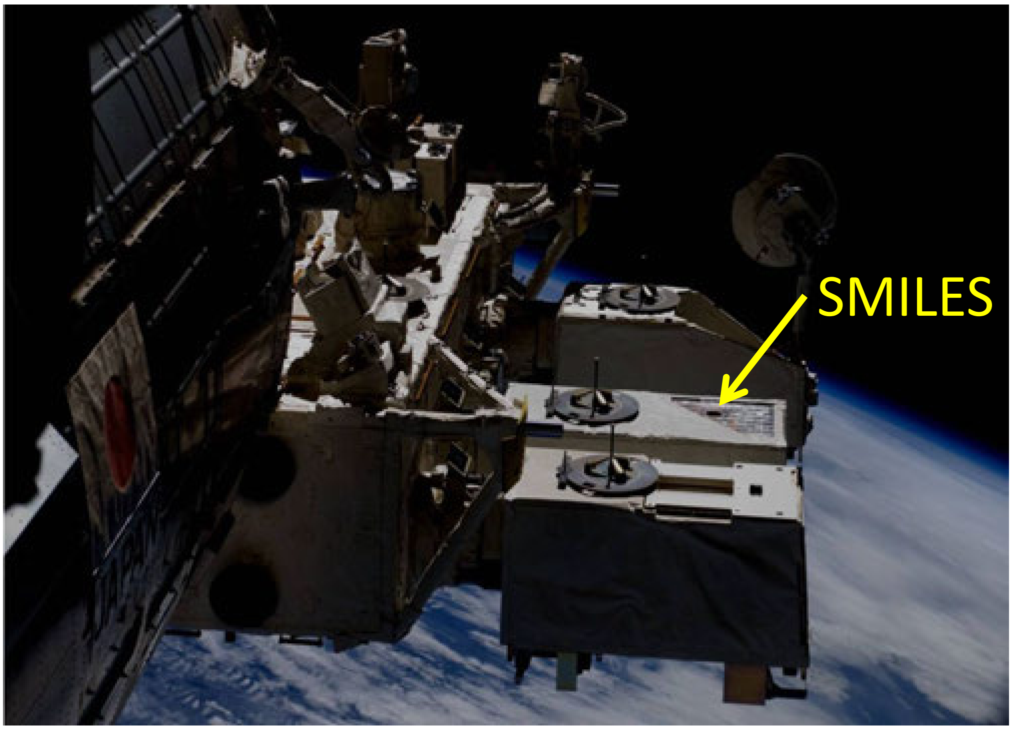
Welcome Address
- Achievement of SMILES Mission -



The International Space Station



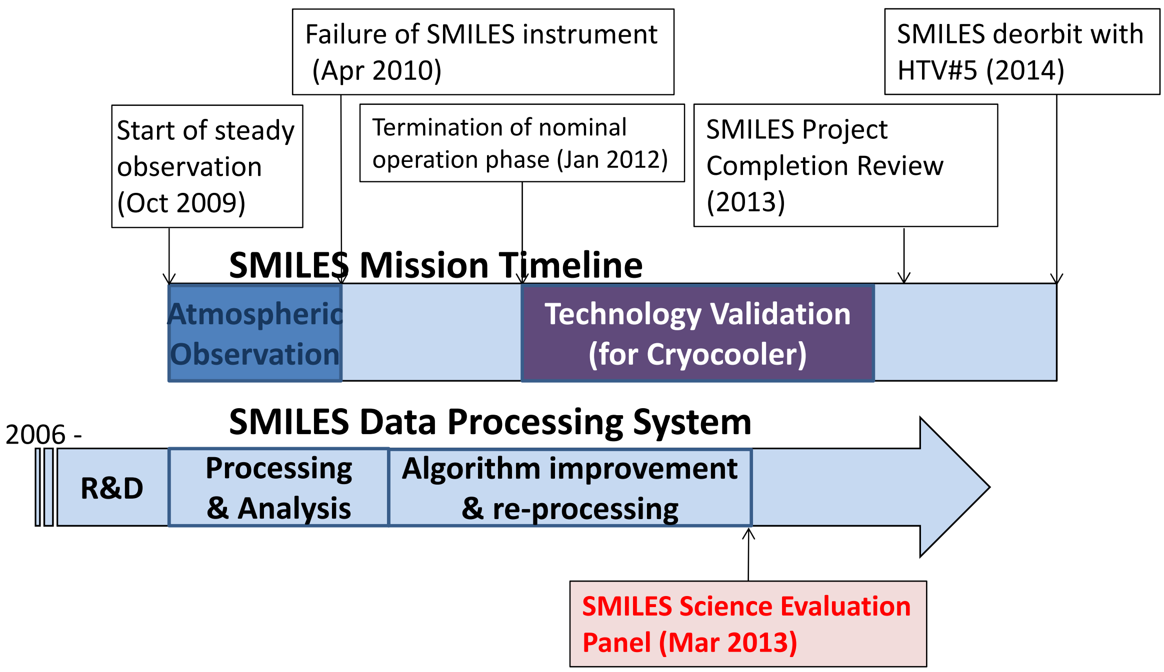
SMILES onboard JEM/ISS



History of SMILES mission

- 1997/4 Selected as 1st-phase mission of Exposed Facility of JEM/ISS
- 2006/5
  - Revision of implementation in JAXA; ISAS has a role in SMILES Science
  - Prof. Shiotani is charged as the Principal Investigator
- 2008/5-8 Research Announcement
- 2009/9 Launch of SMILES / HTV-1 / H-IIB #1
- 2009/10 Start of Atmospheric Observation

Position of the Evaluation Panel in JAXA SMILES project



Cooperation of JAXA and NICT in SMILES mission

JAXA

- Development of some components
- Integration of SMILES instrument
- System test of the instrument
- Launch operation
- On-orbit mission operation
- Calibration and validation
- Level 1 data processing
- **Level 2 data processing**
- **Science team activities**

NICT

- Development of some components (receiver, optical systems, local oscillator, etc.)
- Level 3 data processing (quick look pictures)

The evaluation panel covers the achievement of Level 2 data processing and related studies, which were implemented in ISAS/JAXA.

SMILES Research Announcement

- Announced in May 2009, application closed in July 2009.
- 30 themes have been proposed and 28 of them were accepted.
- Some of applied research activities outside JAXA are provided within the scheme of SMILES RA.

  (Example)
  - Ice cloud retrieval, BrO comparison, etc. (JPL)
  - Level 2 research product, stratospheric wind retrieval, etc. (NICT)
  - Ozone isotope comparison, etc. (Toronto U.)

Evaluation Point of View

(1) Adequecy of Research Target
- Was our research target of SMILES appropriate ?

(2) Research implementation system
- Was implementation system of SMILES research properly established ?

(3) Scientific / Engineering Achievement
- Did we achieve our research target ? How about the degree of achievement ?
- How is significance of the results ?
- Does the result have impacts at international level ?

(4) Knock-on effect to the scientific community
- Are we ready to supply SMILES data to the scientific community to be utilized for their applied researches ?
- Are there sufficient knock-on effect to the related scientific communities ?

Evaluation Panel Members

Chair
- Dr. John C. Gille (NCAR)

Members
- Dr. Guy Brasseur (German Climate Service Center)
- Dr. Paul A. Newman (NASA/GSFC)
- Prof. Emeritus Dr. Toshihiro Ogawa (Univ. of Tokyo)
- Prof. Emeritus Dr. Norio Kaifu (National Astronomical Observatory of Japan)
- Prof. Dr. Hideaki Nakane (Kochi Univ. of Tech.)
- Prof. Dr. Masato Nakamura (ISAS/JAXA)

JEM/SMILES Mission

(JEM/SMILES: Superconducting Submillimeter-Wave Limb-Emission Sounder designed to be aboard the Japanese Experiment Module on ISS; Collaboration project of JAXA - Japan Aerospace Exploration Agency - and NICT - National Institute of Information and Communications Technology -)

1. Demonstration of superconductive mixer and 4-K mechanical cooler for the submillimeter limb-emission sounding in space

[Mechanical Cooler] Two-stage Stirling and J-T; 20mW @4K, 200mW @20K, 1000mW @100K; Power Consumption: <300 W; Mass: 90 kg

[SIS Mixer]
RF: 640 GHz, IF: 11-13 GHz; Junction: Nb/AlOx/Nb, ~7 kA/cm^2; Fabricated at Nobeyama RO

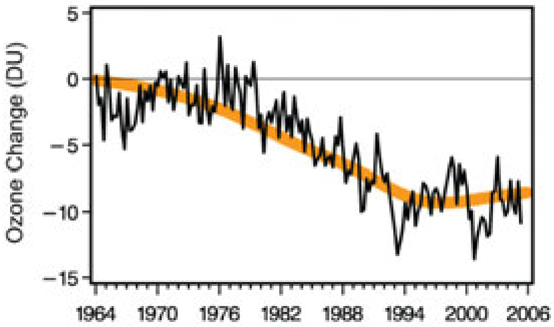
2. Observation on atmospheric minor constituents in the middle atmosphere

[Standard Products]
- 1 scan : O_3, HCl, ClO, CH_3CN, O_3 isotopes, HOCl, HNO_3
- Multi-scan : HO_2, BrO

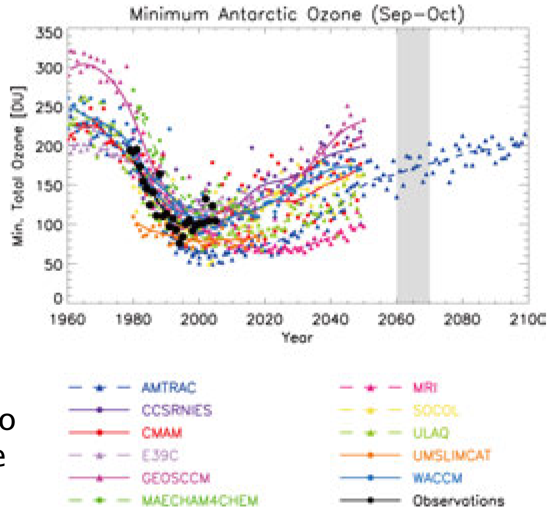
[Research Products] UTH, Cirrus Clouds, volcanic SO_2, H_2O_2

2

Background: Future Ozone Layer



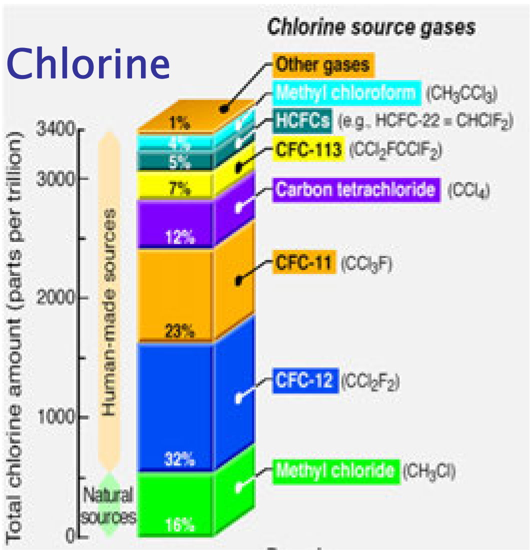
Not only in the polar latitudes, but also in the mid- and lower latitudes, ozone depletion is critical whole the globe. The recovery is estimated around 2060-2070, but there is very big uncertainty in association with the Cl and Br chemistries (WMO, 2006)

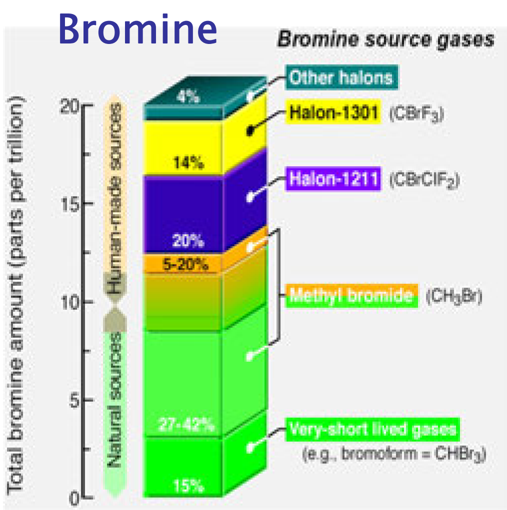


Model results for the future Antarctic ozone amount calculated from chemistry-climate models (WMO, 2006)

3

Origin of Cl and Br in the Stratosphere





Our quantitative understanding of how halogenated very short-lived substances contribute to halogen levels in the stratosphere has improved significantly since the 2002 Assessment, with brominated very short-lived substances believed to make a significant contribution to total stratospheric bromine and its effect on stratospheric ozone. (WMO Ozone Report, 2006)

4

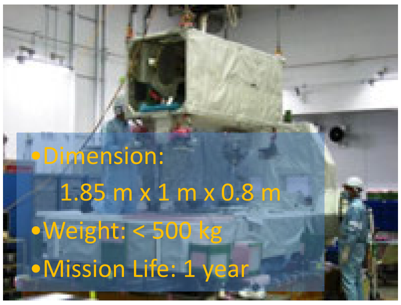
Scientific targets of SMILES

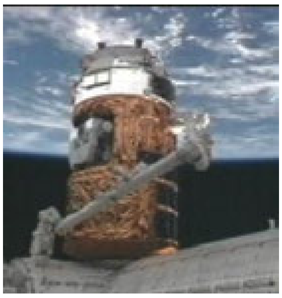
1. Inorganic Chlorine chemistry
   - ClO to HCl ratio (O$_3$ trend in the US)
   - HOCl production (O$_3$ trend in the LS)
   - Global ClO (background ClO)
2. Bromine budget (very short-lived source gas)
3. HO$_x$ budget (HO$_x$ dilemma)
4. Cirrus clouds (Het. reactions & rad. budget)
5. O$_3$ isotope (mass independent chemistry)

(6. UT/LS mixing (O$_3$ flux))

5

JEM/SMILES payload and status





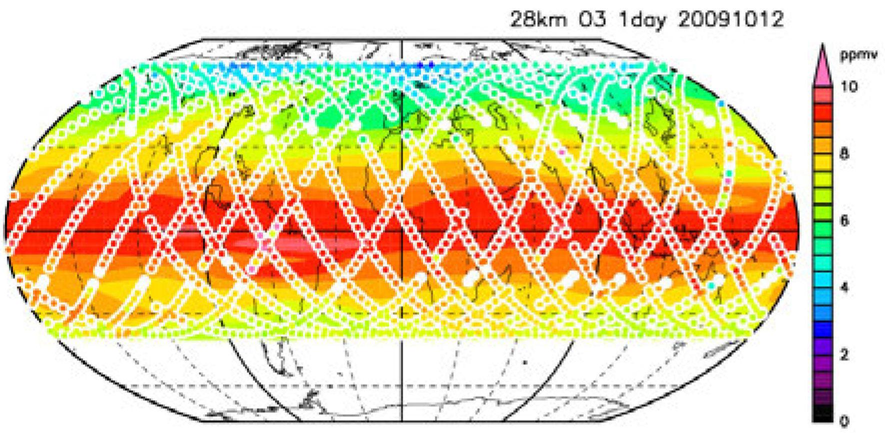
- Sep. 11, 2009: SMILES was carried by H-IIB with H-II Transfer Vehicle (HTV)
- Sep. 18: HTV was attached to ISS ; Sep. 25: SMILES was attached to JEM
- Sep. 28: The cooler reached 4K
- Oct. 12: Continuous observations started

- Apr. 21, 2010: SMILES observations have been suspended due to the failure of a critical component in the submillimeter local oscillator.
- June 5: The cooler stopped its operation due to the failure of the JEM thermal control system.
- Jan 19, 2011: JAXA officially announced termination of the normal operation (All dates in JST)

6

SMILES measurements

- High sensitivity in detecting atmospheric limb emission of the submillimeter wave range; Band-A : 624.32- 625.52GHz, Band-B : 625.12- 626.32GHz, Band-C : 649.12- 650.32GHz
- Vertical profiling (about 3km resolution) from ISS with latitudinal coverage of 65N to 38S; 53 sec for one sequence, about 100 points per one orbit, and about 1600 points per day.
- SMILES can measure the atmosphere at different local times because of the non-sun-synchronous ISS orbit.

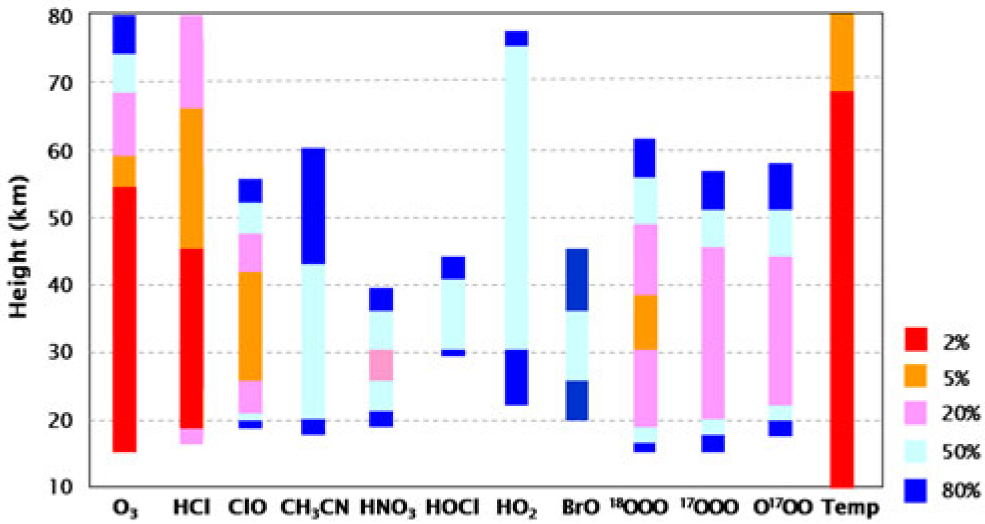


Globally mapped ozone distributions at 28 km on October 12, 2009. Original observation points are plotted by white circles with observed ozone mixing ratios.

7

SMILES observation performance

Measurements on several radical species crucial to the ozone chemistry (normal O_3, isotope O_3, ClO, HCl, HOCl, BrO, HO_2 ...)

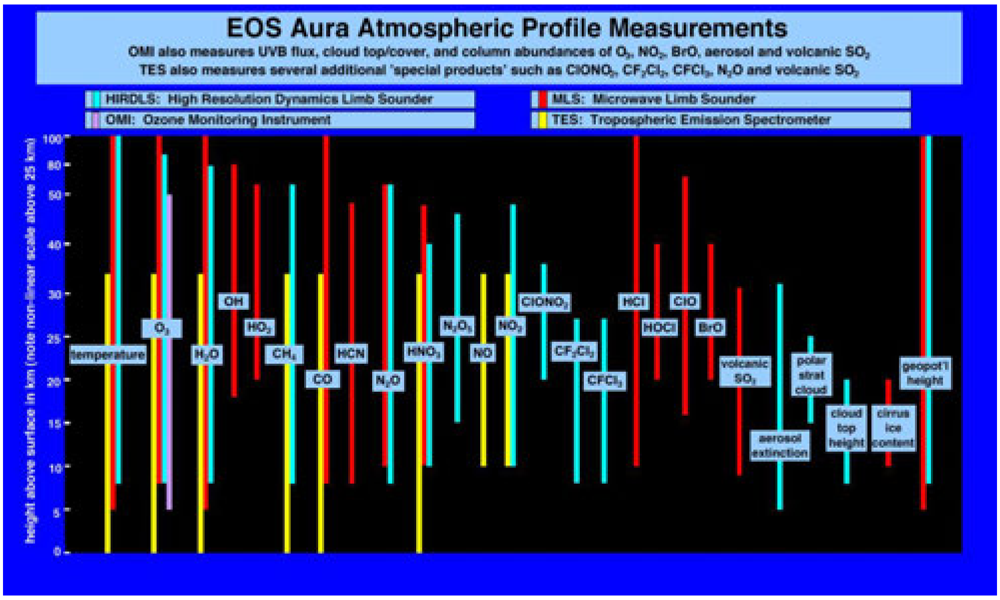


Error estimation for the mid-latitude case based on the single scan measurement

8

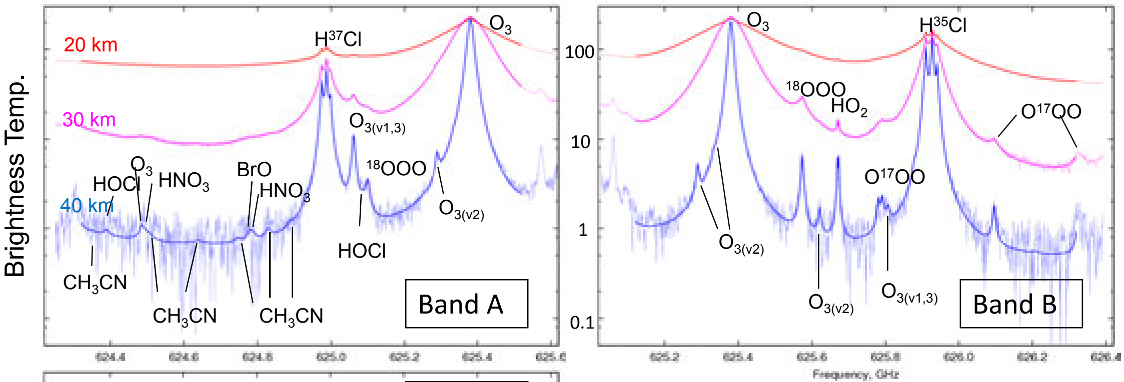
Cf. EOS Aura measurements

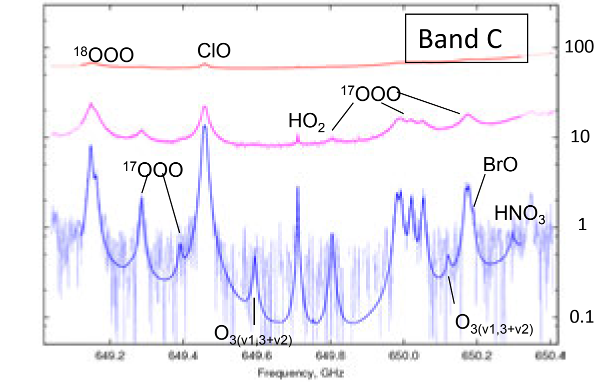
EOS-Aura launched in July 2004



9

Typical day-time spectra

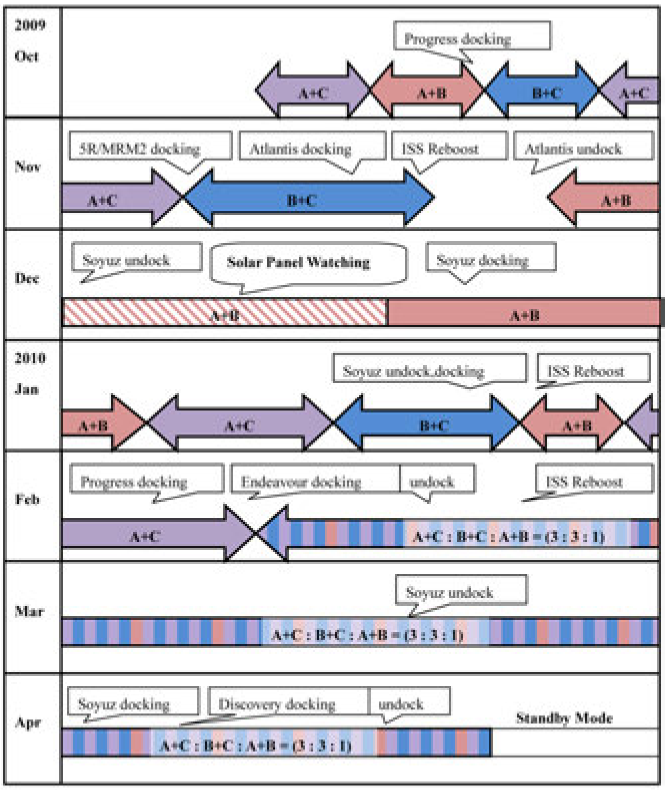




Observed spectra are in thin lines and fitted spectra are in thick lines

10

Status of SMILES observation



Two bands out of the three are used

11

Operational Level 2 products

- v1.0 (005-06-0024): for retrieval test (2010/01/23 released)
- v1.1 (005-06-0032): for mapping test (2010/04/19 released)
- v1.2 (005-06-0150): algorism update I (2010/09/15 released)
- v1.3 (006-06-0200): algorism update II (2011/03/02 released)
- v2.0 (007-08-0300): major update (2011/10/04 released)
- v2.1 (007-08-0310): improvement in HOCl (2012/01/16 released)
  - Public release (2012/03/05)
- v2.2 (007-09-0400): algorithm update
- v2.3 (007-09-0402): minor update
- v2.4 (008-11-0502): a priori profile update

http://smiles.isas.jaxa.jp/access/indexe.shtml

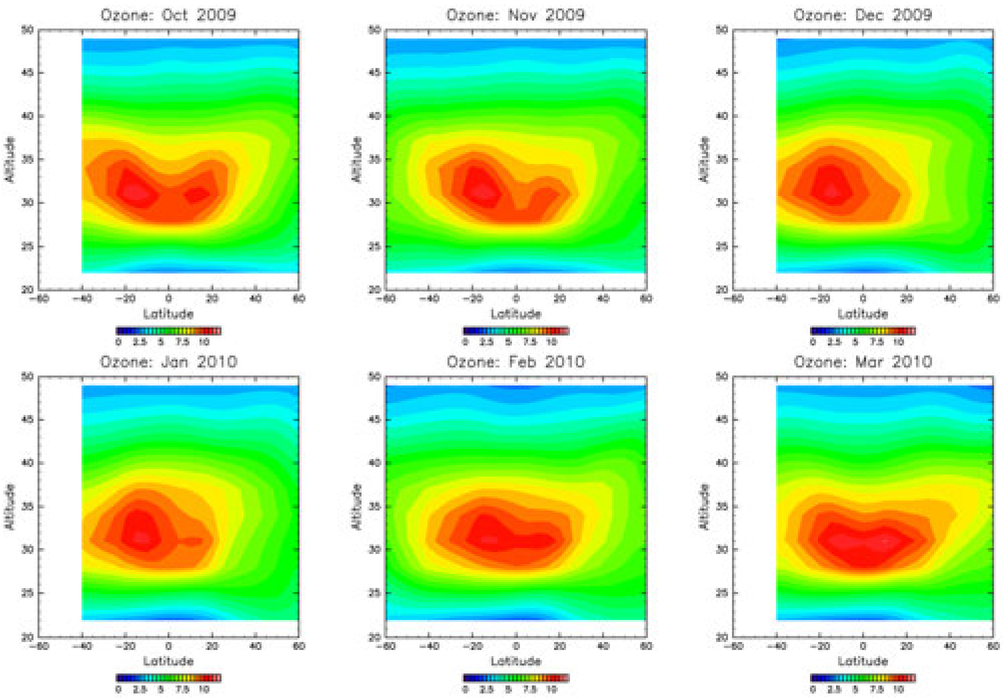
12

General pictures during the SMILES observation period:

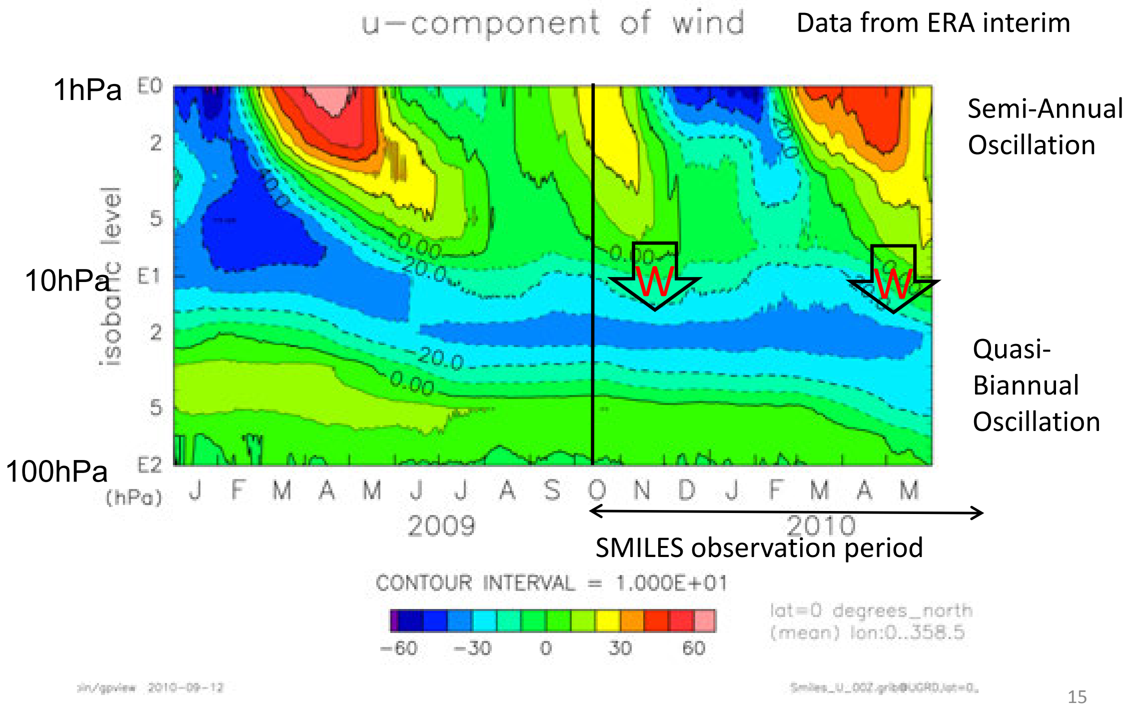
i) seasonal evolutions in the equatorial latitudes

ii) a stratospheric sudden warming in Jan 2010

Seasonal evolution of ozone



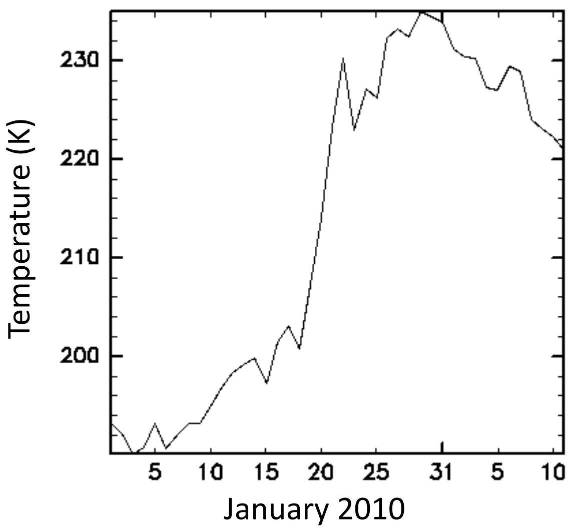
Time-height section of zonal wind (EQ)

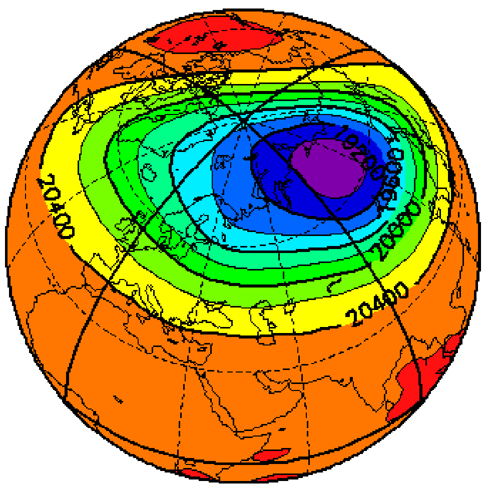


15

A stratospheric sudden warming in January 2010

NP temperature at 10hPa

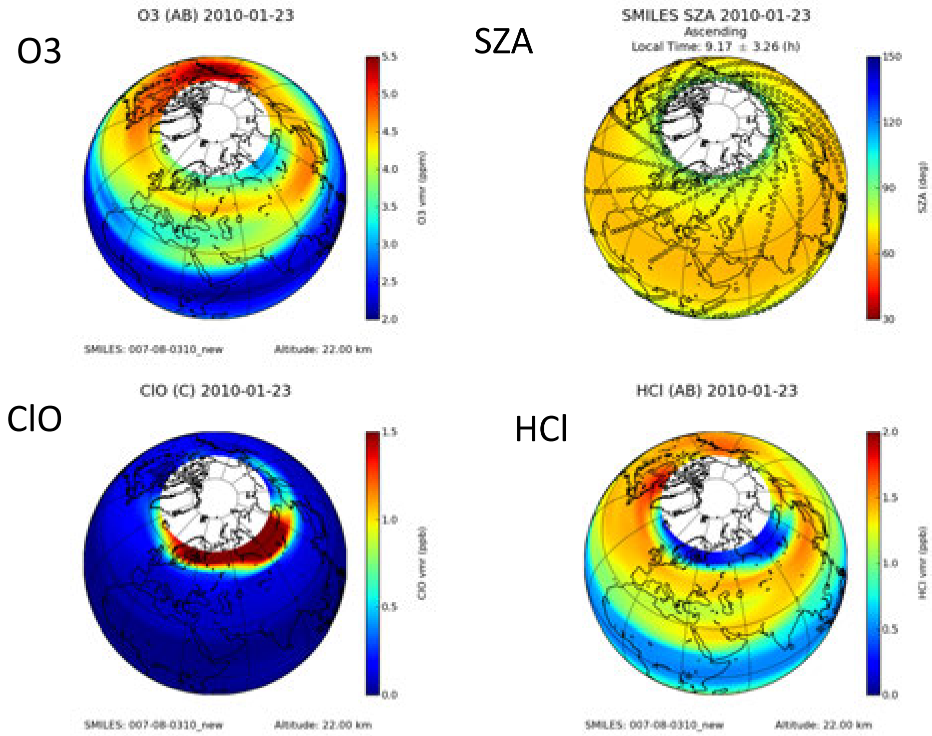




GP height field at 50 hPa on January 23

16

Time evolution in January 2010



17

Diurnal ozone variations in the stratosphere revealed in observations from the Superconducting Submillimeter-Wave Limb-Emission Sounder (SMILES) onboard the International Space Station (ISS)

by Sakazaki et al.
(accepted, JGR)

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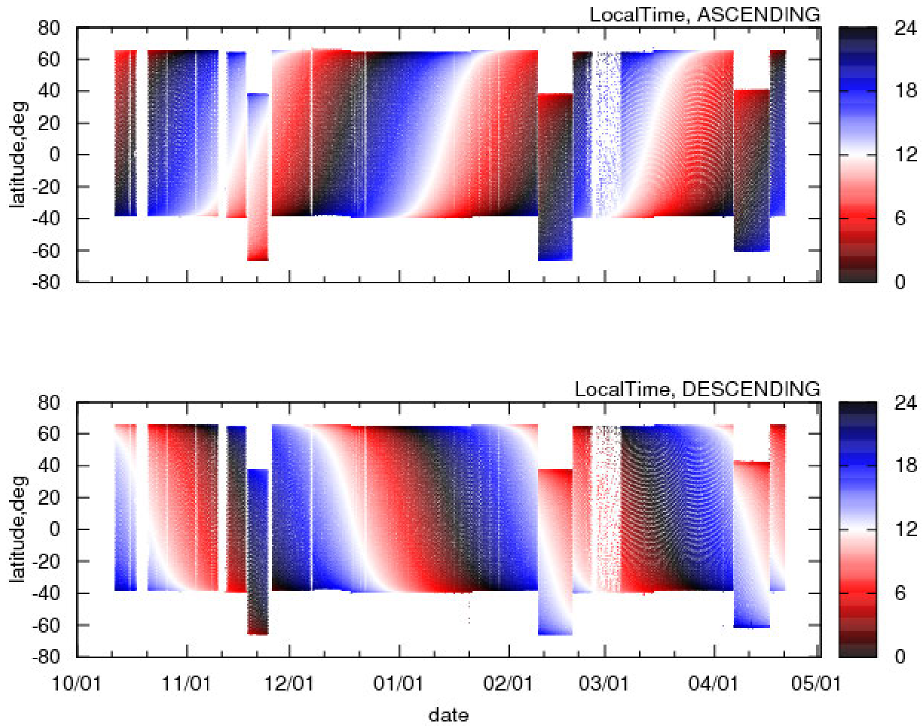
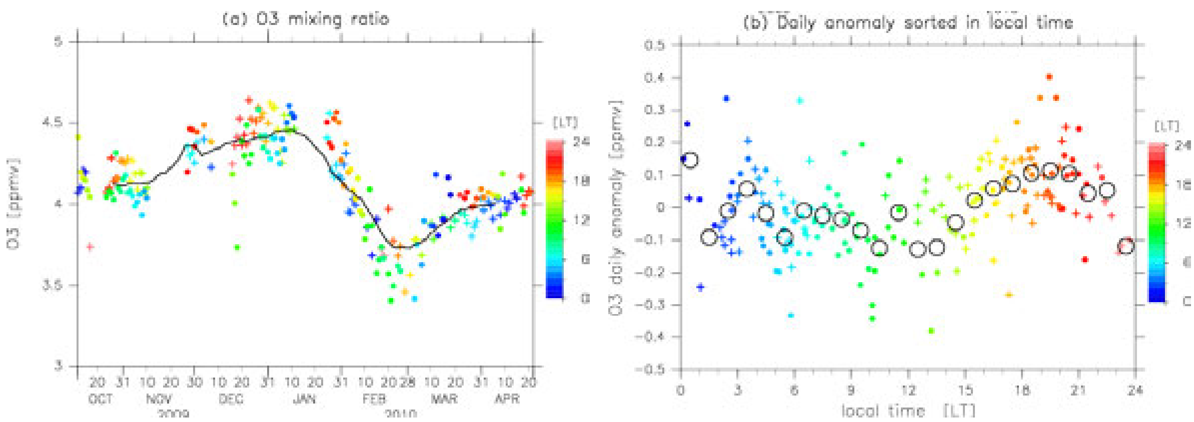
Local time variations

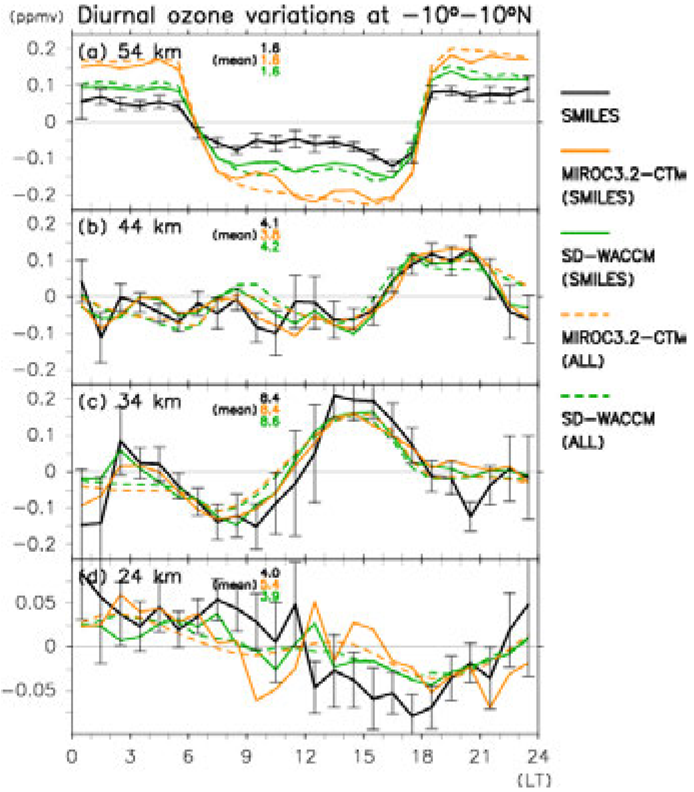


Daily time series and the residual from the 30-day running mean



Daily time series of ozone mixing ratio at the equator averaged over the longitude at an altitude of 44 km.

Diurnal variations averaged over 10S-10N



SD-WACCM

- Specified Dynamics (SD) version of WACCM
- Whole Atmosphere Community Climate Model
- Temperature and wind fields from NASA GEOS5.1 are nudged
- horizontal : 1.9°x2.5°, vertical: 88 levels (up to 140km)
- 57 species (Ox, NOx, HOx, ClOx, BrOx etc.)
- 230 chemical reactions

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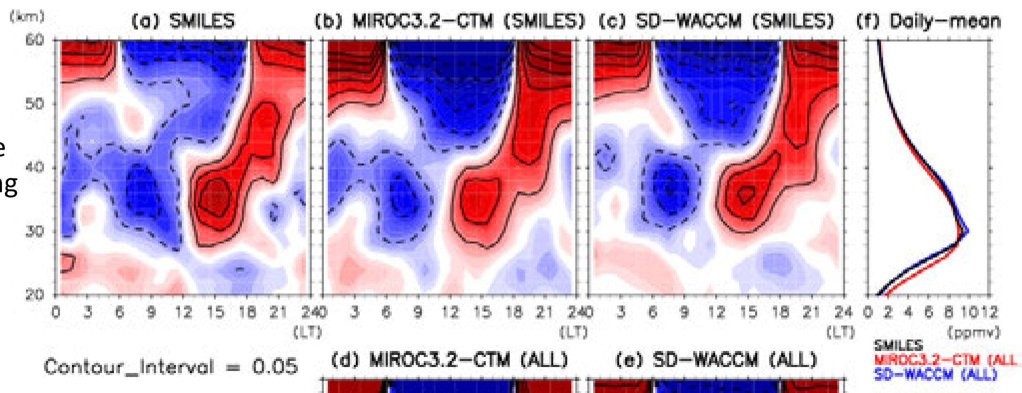
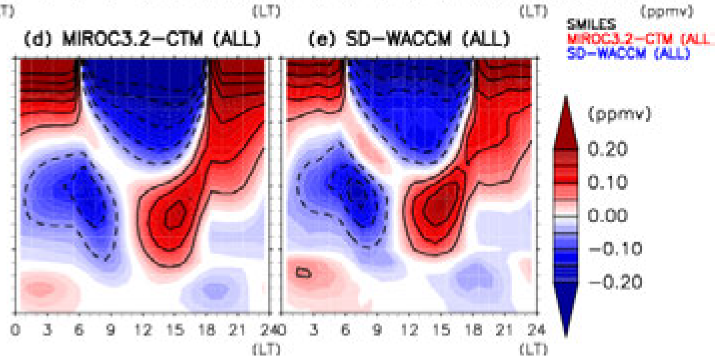
Diurnal variations in ozone

Satellite sampling





Diurnal amplitude
20–30 km: 0.05 ppmv (1%)
30–40 km: 0.15 ppmv (2-3%)
40–50 km: a minimum of 0.1 ppmv (3-4%) at about noon, and a maximum of 0.1 ppmv (3-4%) in the late afternoon

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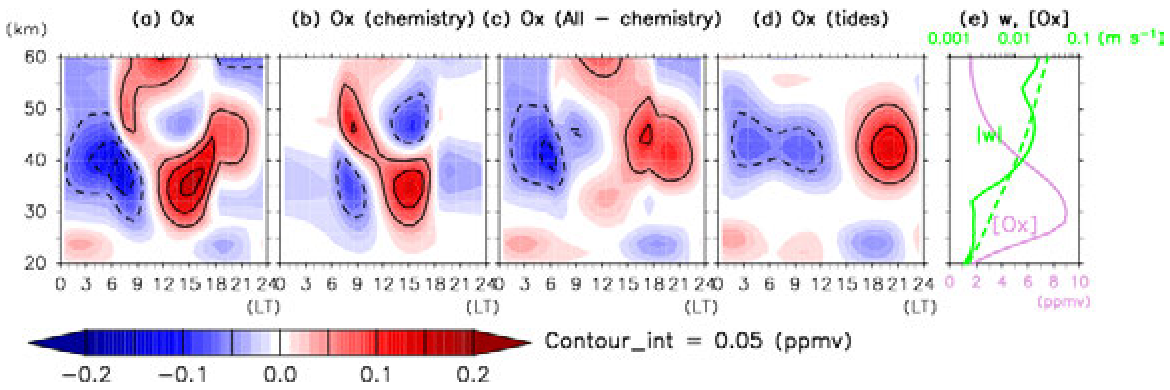
Mechanism of the diurnal variations



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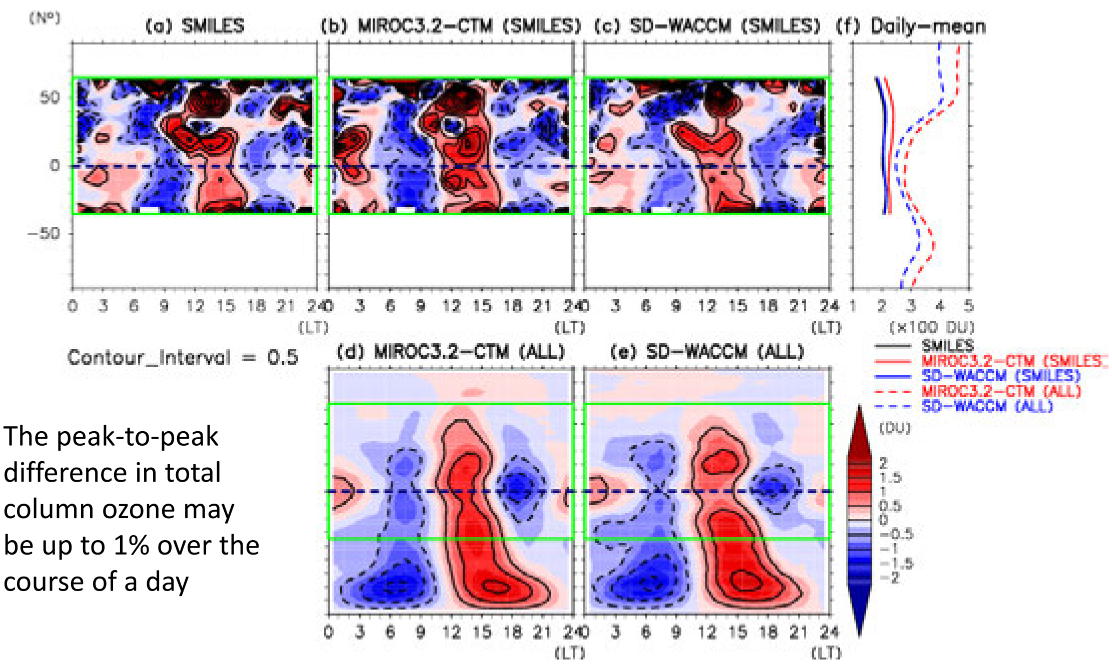
Diurnal variations in total ozone



The peak-to-peak difference in total column ozone may be up to 1% over the course of a day

- A bias in the SAGE sunrise and sunset profiles [McLinden et al., 2009]
- Orbital drift of SBUV onboard NOAA satellites [Wang et al., 2012]
- TOMS and OMI measurement local times are 1130 LT and 1330 LT

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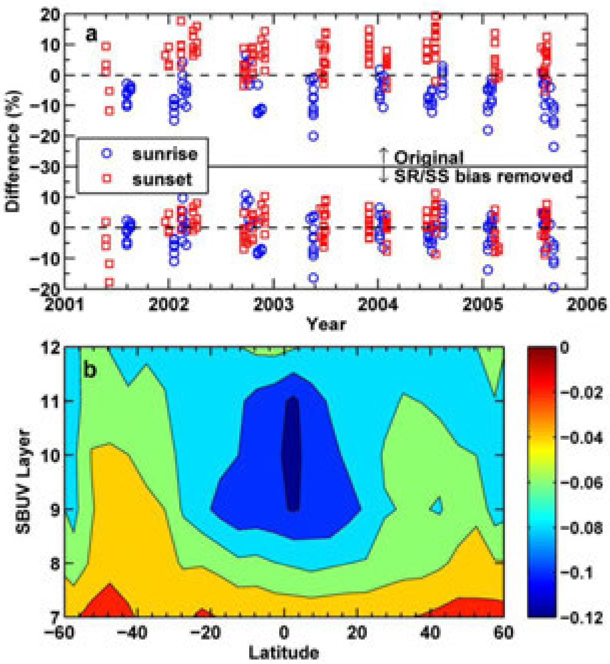
SAGE sunrise & sunset bias

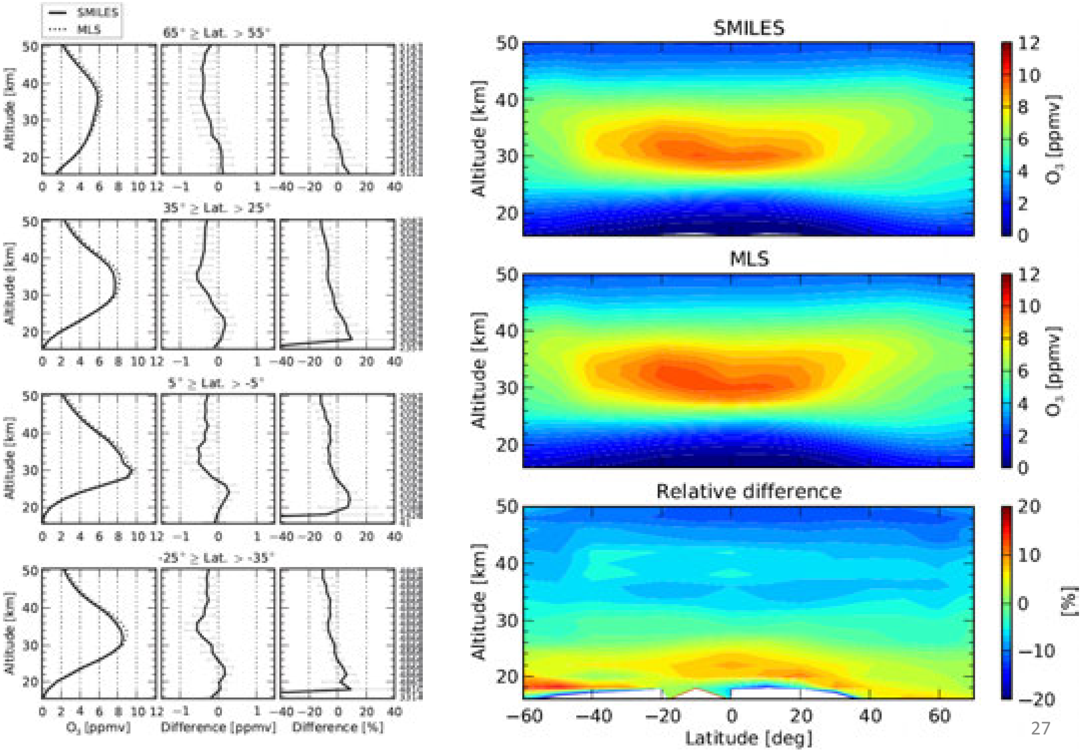


(upper) Relative difference between SAGEII and NOAA16/SBUV2 ozone partial columns in layer 10 at 0-5N before and after the sunrise/sunset (SR/SS) bias was removed.
(lower) SR/SS bias
(McLinden et al., 2009, ACP)

Validation of ozone data from the Superconducting Submillimeter-Wave Limb-Emission Sounder (SMILES)

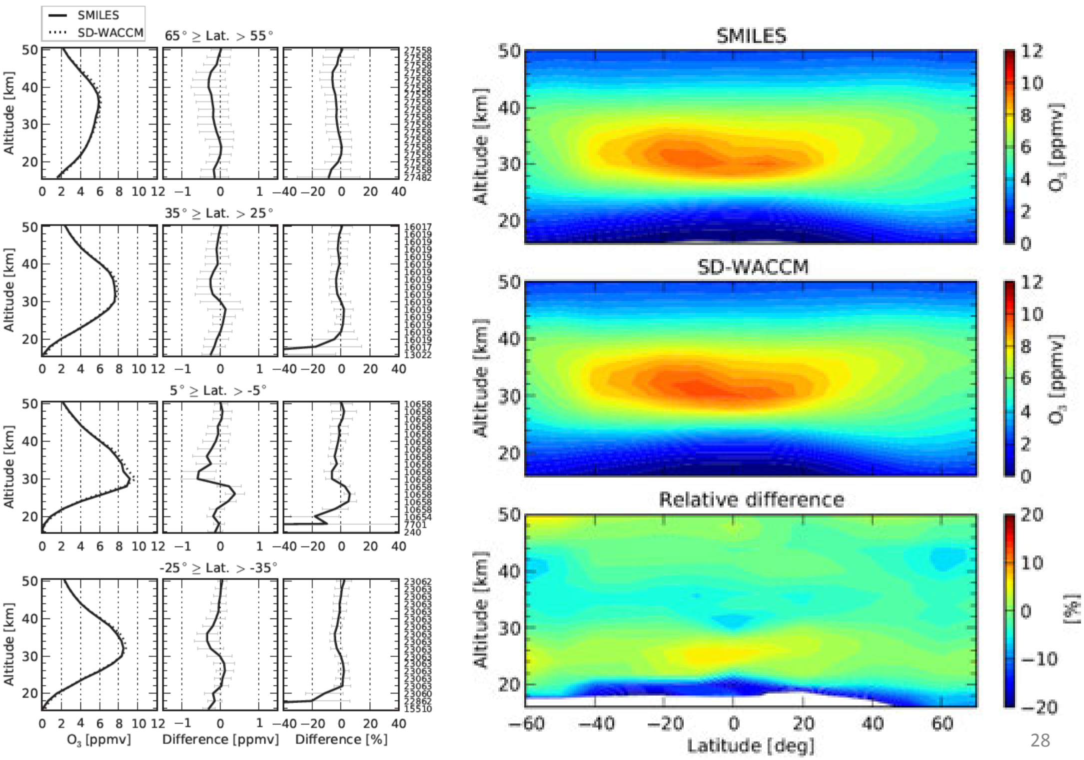
by Imai et al.
(under revision, JGR)

SMILES and MLS comparisons



27

SMILES and SD-WACCM comparisons



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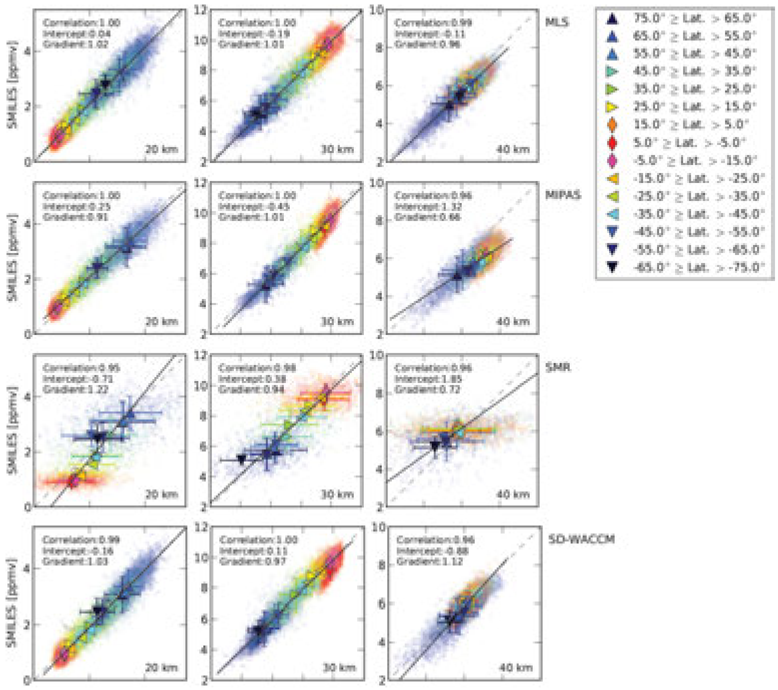
Variability of SMILES ozone data



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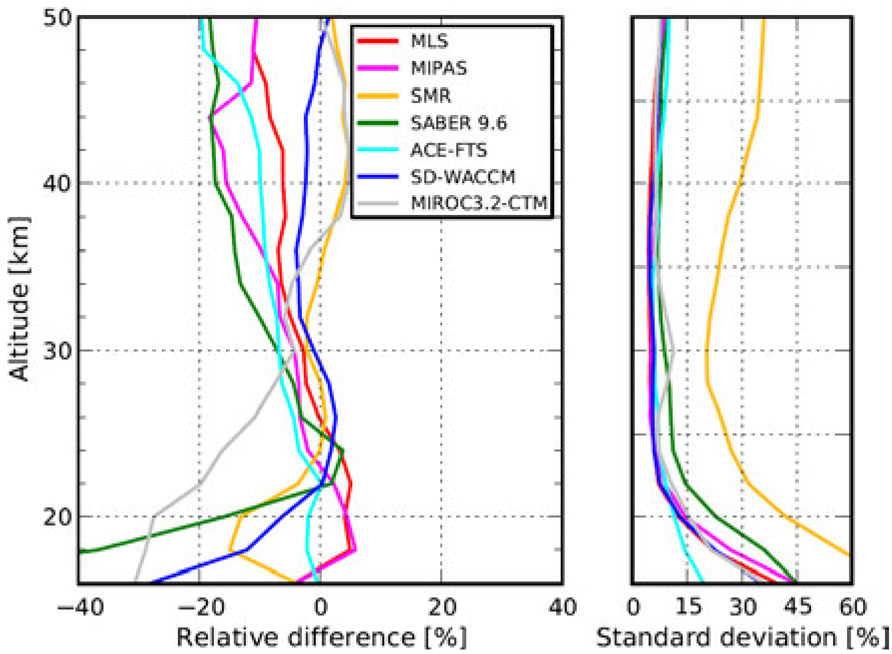
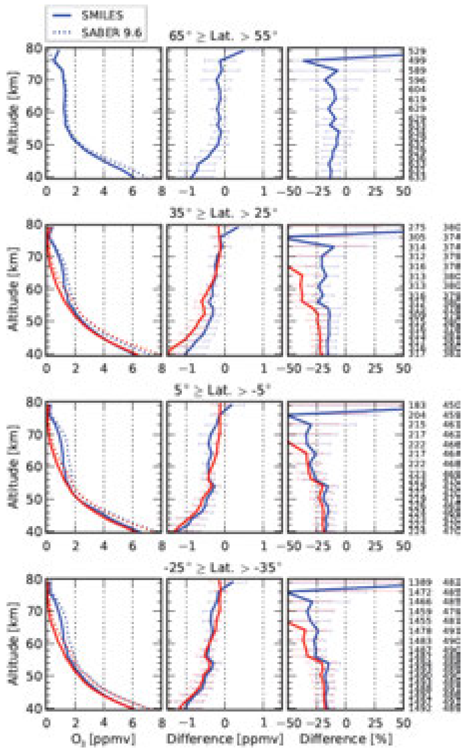
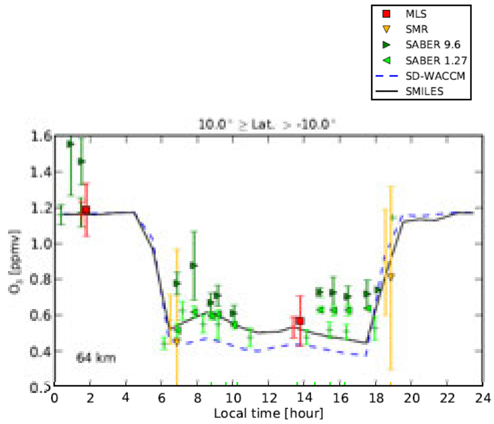
Comparisons of ozone with other data



30

Comparisons in the mesosphere





In details for the mesosphere, see Smith et al., and for the diurnal variations, see Sakazaki et al.

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Comparison of ozone profiles between Superconducting Submillimeter-Wave Limb-Emission Sounder (SMILES) and worldwide ozonesonde measurements

by Imai et al.
(submitted to JGR)

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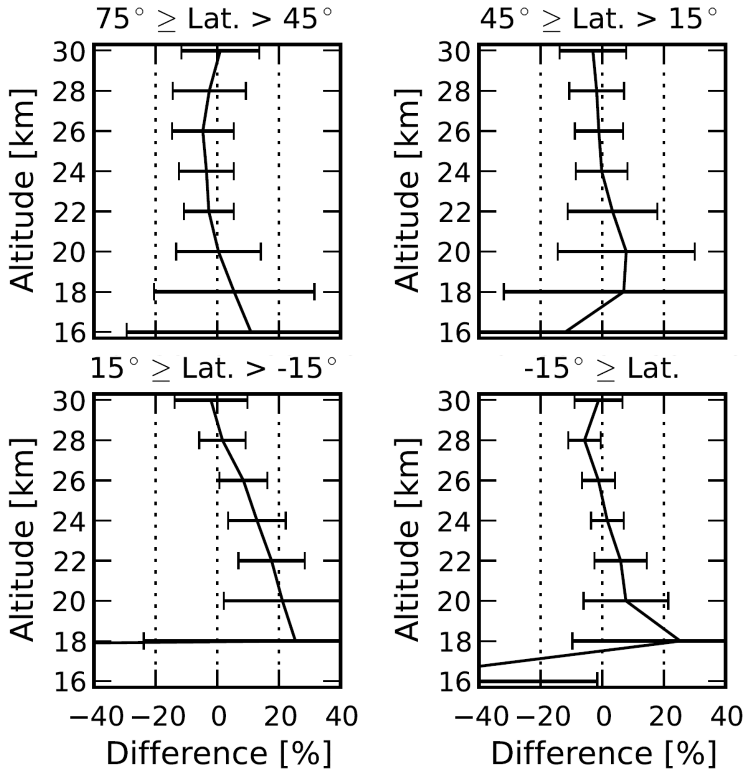
Comparisons with ozonesondes



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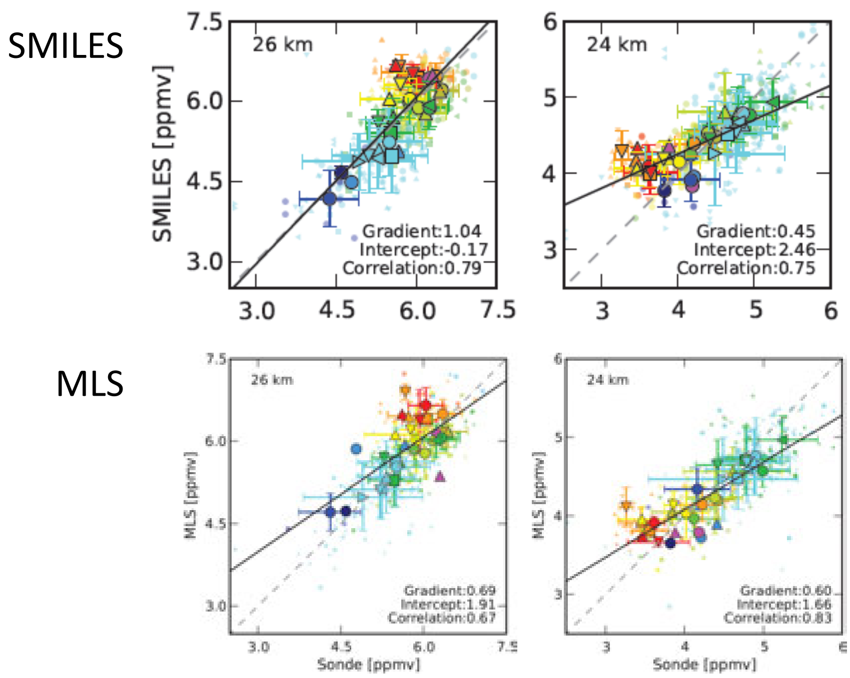
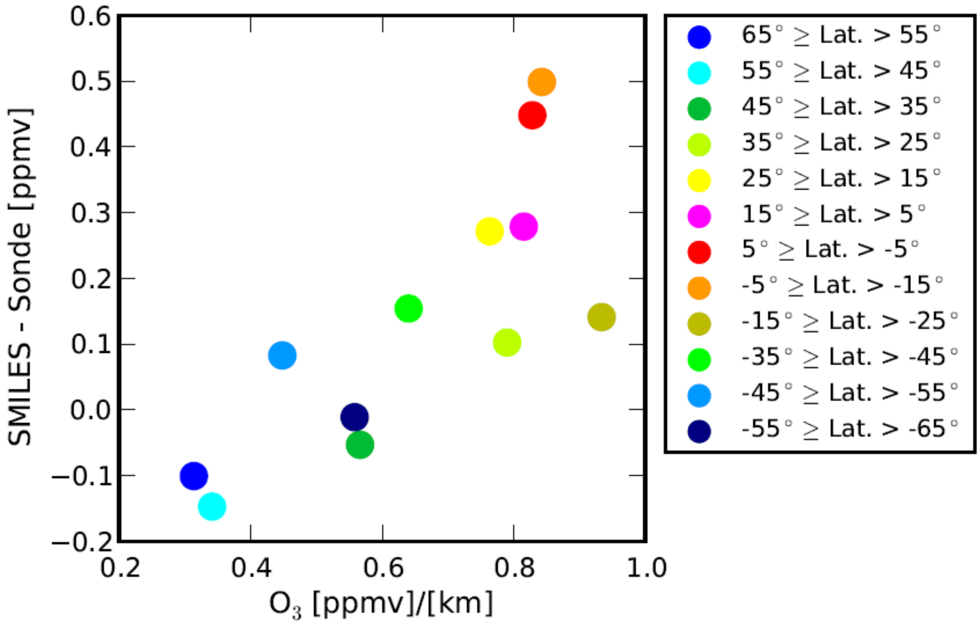
Latitudinal structure – SMILES & MLS



34

Relation between vertical gradient and differences (SMILES – ozonesonde)



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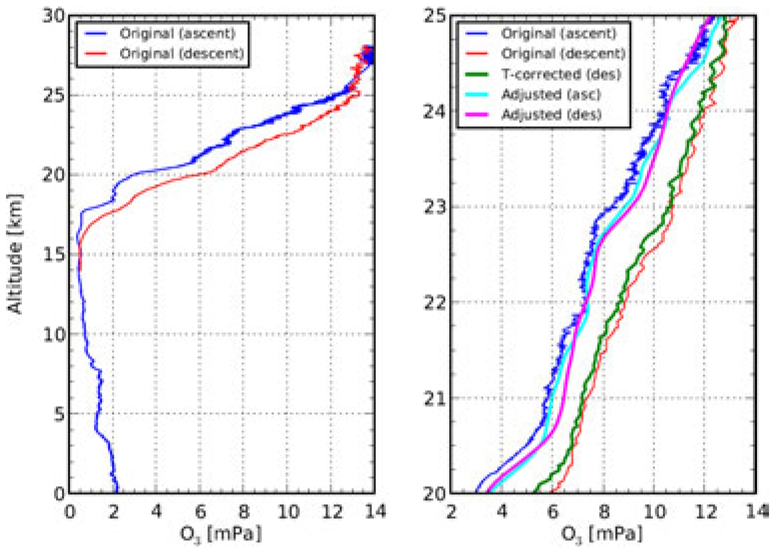
Ozonesonde measurements with ascending and descending profiles



A time-lag correction proposed by Miloshevich et al. [2004] for humidity measurements of radiosondes

$$\frac{dX_m}{dt} = k(X_a - X_m)$$

$$X_m(t) = X_a - [X_a - X_m(t_0)]e^{-\Delta t/\tau}$$

The ozonesonde's response time is assumed to be within 20–30 s [e.g. Smit et al., 2007]), and our estimation showed response times around 28 s.

By applying this correction to the original profiles, we found a negative bias of the ozonesonde measurement more than 7% at 20 km in the equatorial latitude where the vertical gradient of ozone is steep.

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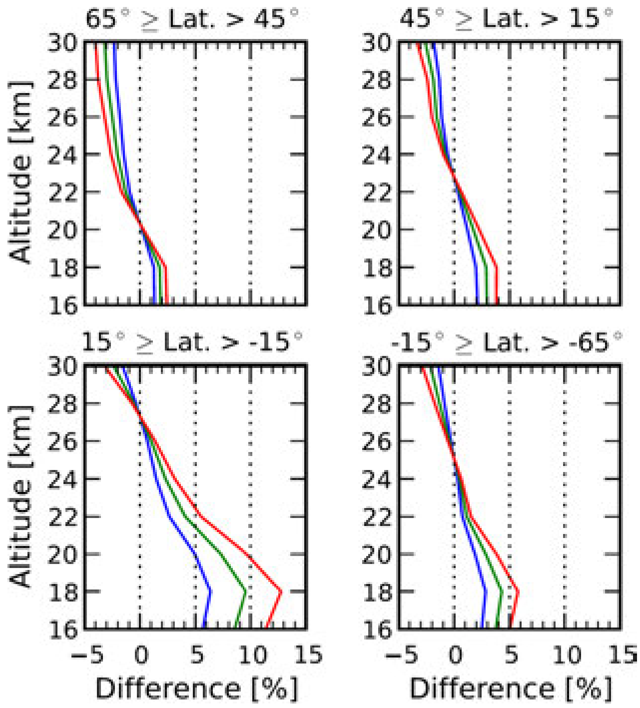
Correction factors of the time-lag effect

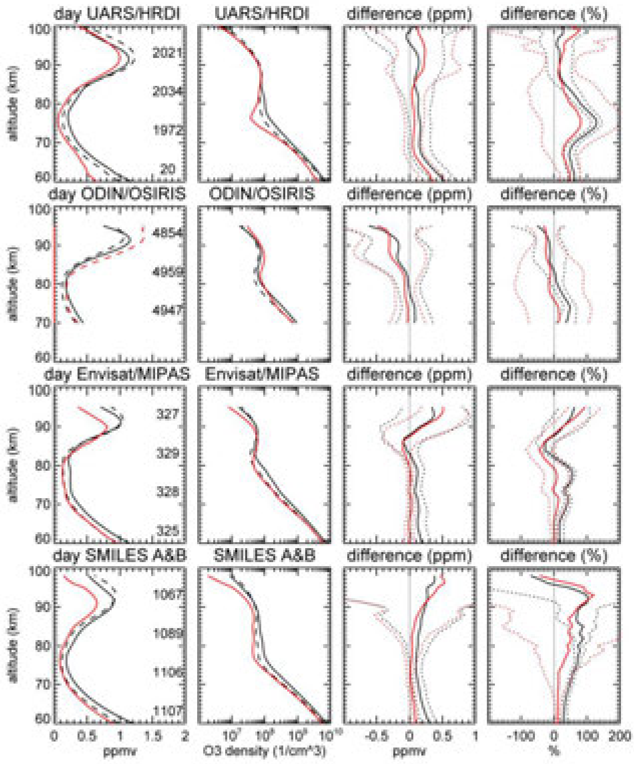


Correction factors with response times of 20 s (blue), 30 s (green) and 40 s (red)

Satellite Observations of Ozone in the Upper Mesosphere

by Smith et al.
(under revision, JGR)

Profiles of daytime ozone



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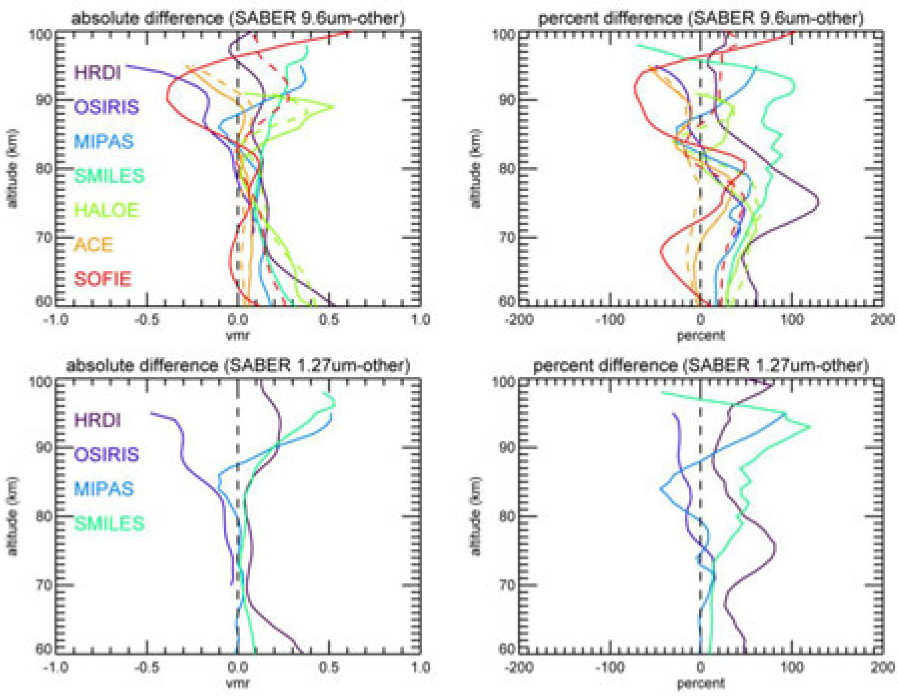
Comparisons with other satellite data



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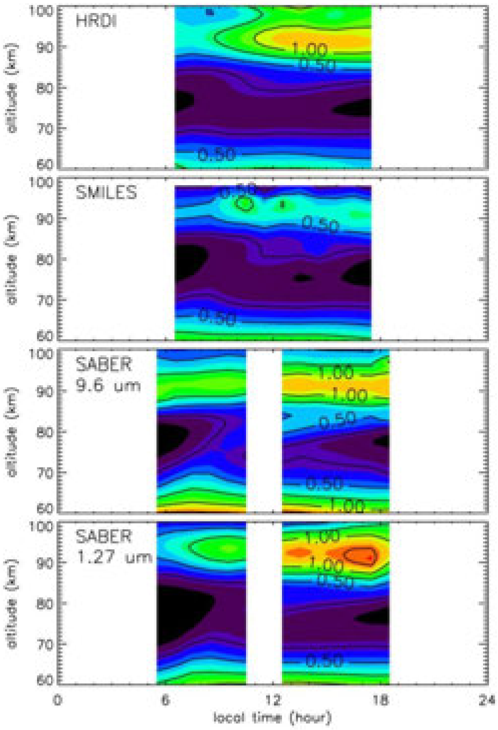
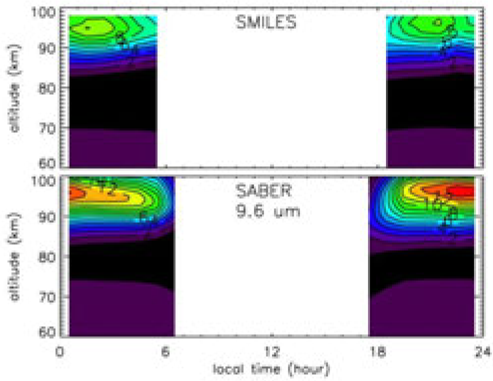
Diurnal variations of mesospheric ozone





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An intercomparison study of isotopic ozone profiles from the ACE, JEM-SMILES, and Odin-SMR instruments.

by Jones et al.
(to be submitted, JGR)

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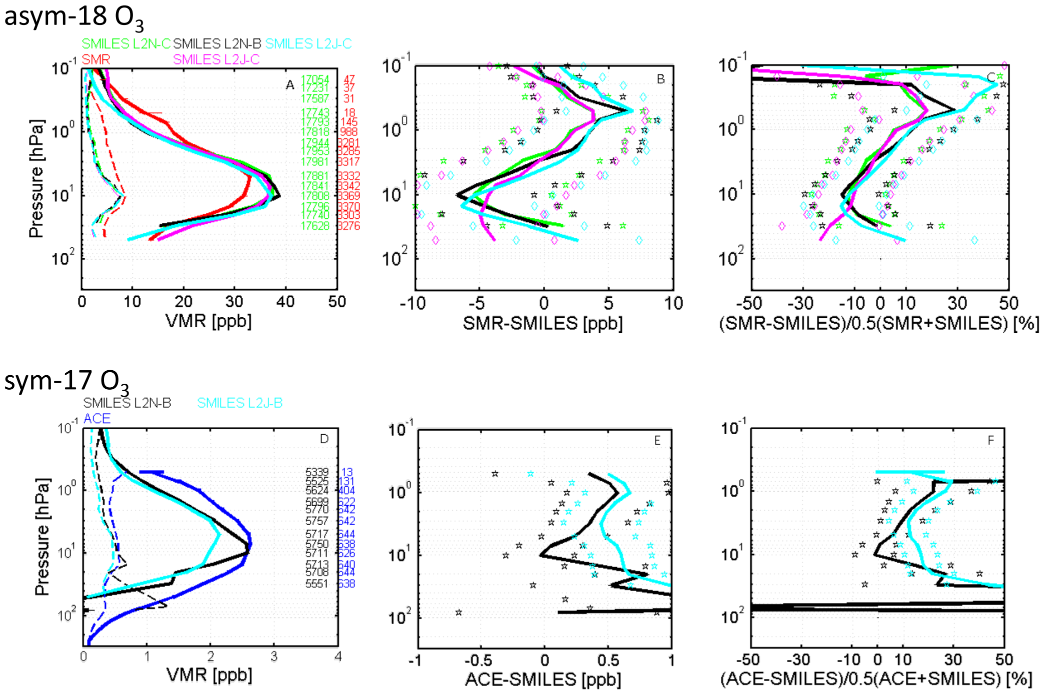
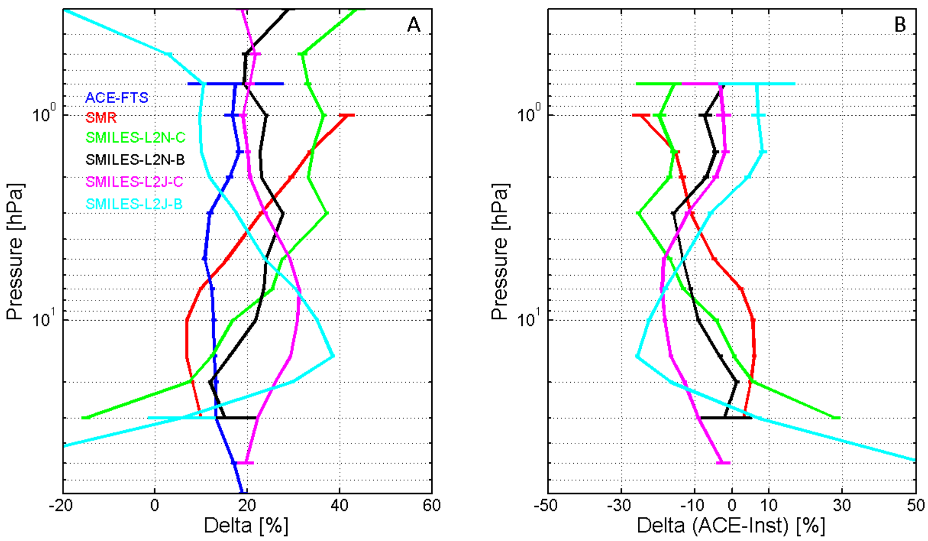
Comparisons for ACE and SMILES



Average asym-18 O_3 enrichment



Summary of results

				Species enrichment ± 1 sigma precision / 1 std (%)				
Platform	Reference	Altitude range (km)	Latitude coverage	Asym-18	Sym-18	Asym-17	Sym-17	$^{50}O_3$
FIRS-2	Johnson et al [2000]	25 - 35	30N - 35N, 68N	12.2 ± 1.0	6.1 ± 1.8	8.0 ± 5.2	1.6 ± 7.6	10.2 ± 0.9
ATMOS	Irion et al [1996]	25 - 40	80S - 80N	15.0 ± 6.0	10 ± 7.0			13.0 ± 5.0
Ground	Meier et al [1996]	Total column	79N	13.5 ± 4.0	11.9 ± 0.9			13.0 ± 2.7
Balloon	Haverd et al [2005]	25 - 35	35N, 65N, 68N	13.5 ± 2.7	7.7 ± 2.2			11.6 ± 2.0
Balloon	Kronkowsky et al [2001]	22 - 33	43N, 68N					7 - 11 (%)
Balloon	Mauersberger et al [2001]	22 - 34	32N, 34N, 43N, 68N					9.0 ± 0.4
Cryosampler/Lab	Mauersberger et al [1993]	25 - 35						11.8 ± 1.0
ACE		25 - 40	30N - 50N	12.3 ± 0.2/0.9	8.8 ± 0.2/0.4		9.4 ± 0.5/2.3	11.1 ± 0.2
SMILES L2N-C		25 - 40	30N - 50N	21.1 ± 0.3/11.1		17.9 ± 0.2/3.8		
SMILES L2N-B		25 - 40	30N - 50N	20.9 ± 0.1/5.8				
SMILES L2-C		25 - 40	30N - 50N	28.4 ± 0.1/2.9		23.3 ± 01./3.3		
SMILES L2-B		25 - 40	30N - 50N	29.3 ± 0.1/7.6				
Odin SMR		25 - 40	30N - 50N	11.7 ± 0.2/6.4	14.5 ± 0.4/0.3	14.5 ± 1.0/8.0*		12.6 ± 0.2

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Validation of ClO data from the Superconducting Submillimeter-Wave Limb-Emission Sounder (SMILES)

by Suzuki et al.
(to be submitted, JGR)

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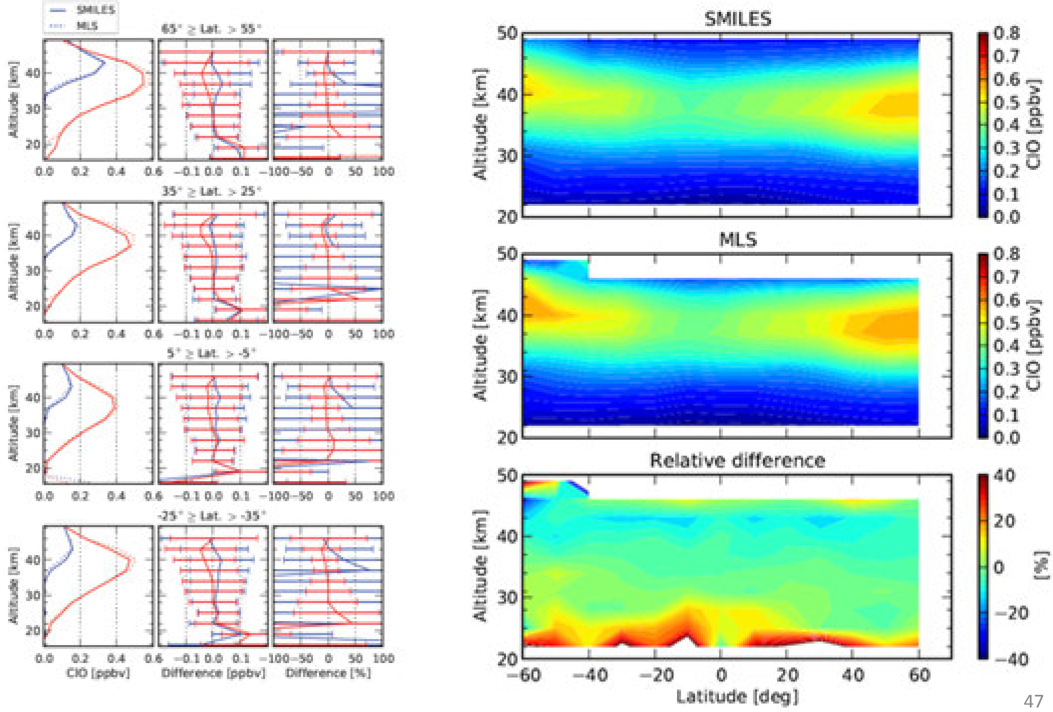
SMILES and MLS comparisons



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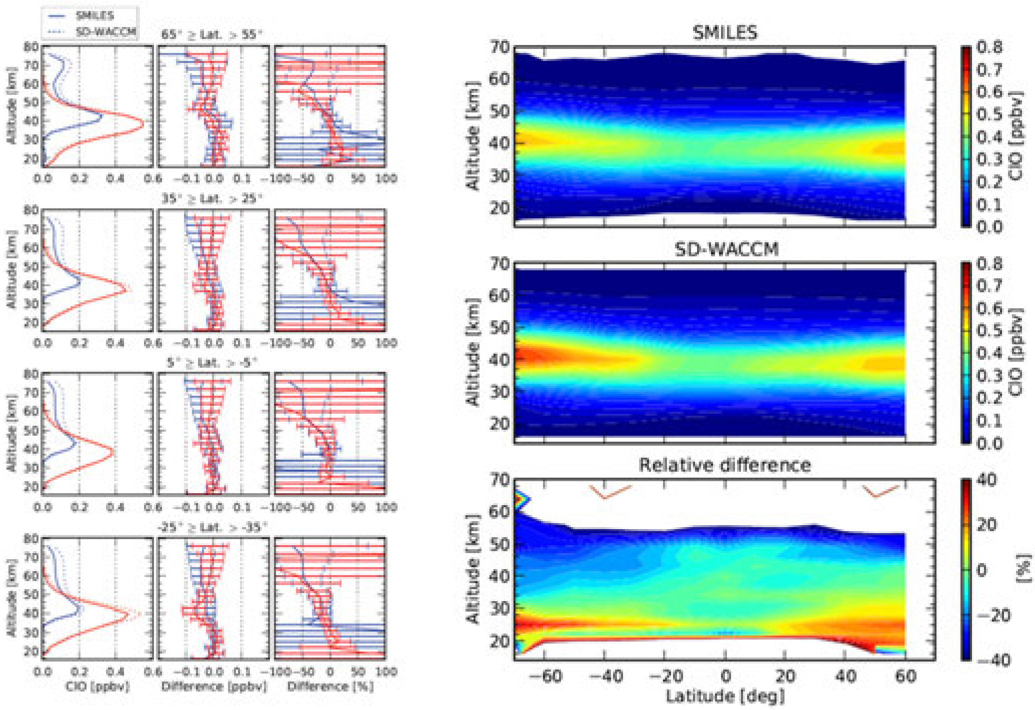
SMILES and SD-WACCM comparisons



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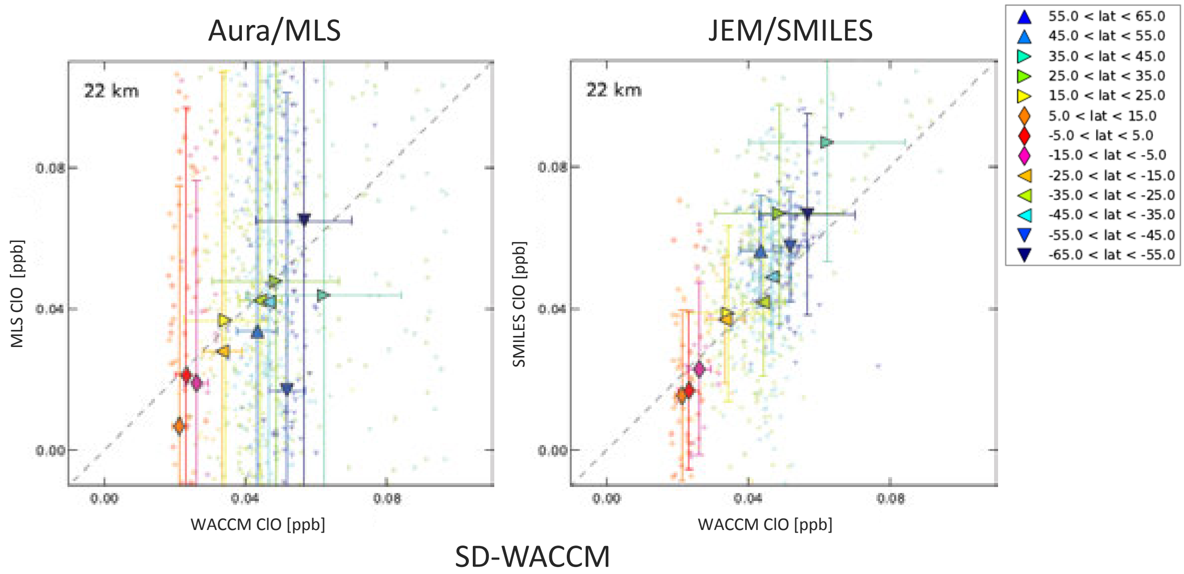
Comparison of SD-WACCM with MLS and SMILES - daytime ClO -



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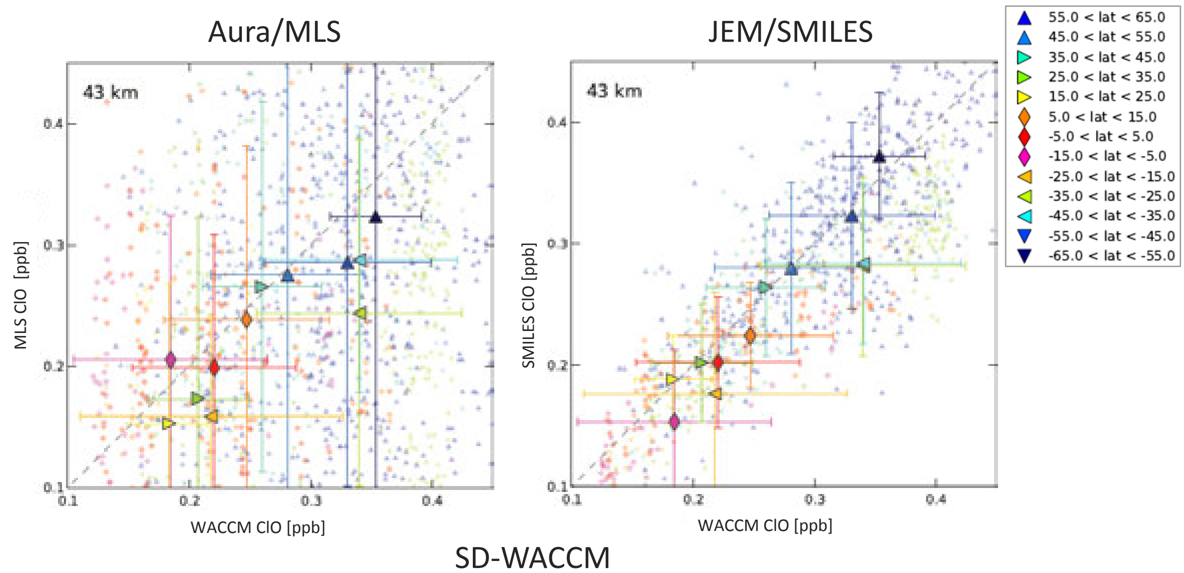
Comparison of SD-WACCM with MLS and SMILES - nighttime ClO -



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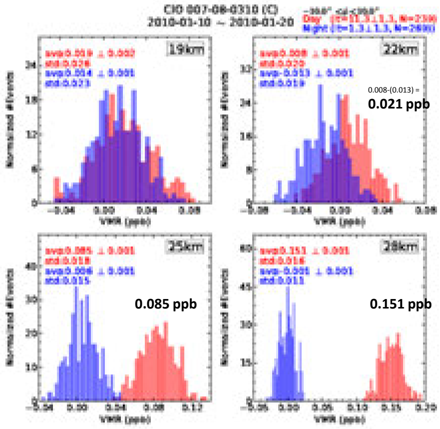
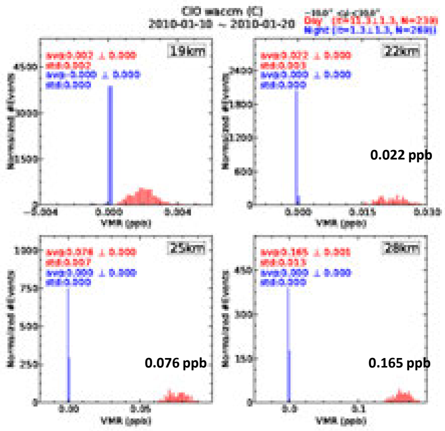
ClO in the Equatorial lower stratosphere

SMILES



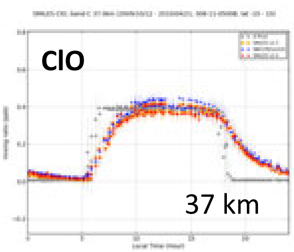
SD-WACCM

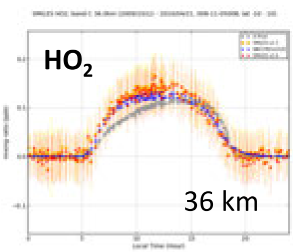


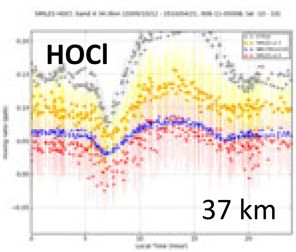
	SMILES			SD-WACCM		
	Day	Night	Day-Night	Day	Night	Day-Night
22 km	8±1	-13±1	21±2	22	0	22
25 km	85±1	6±1	79±2	76	0	76
28 km	151±1	-1±1	152±2	165±1	0	165±1

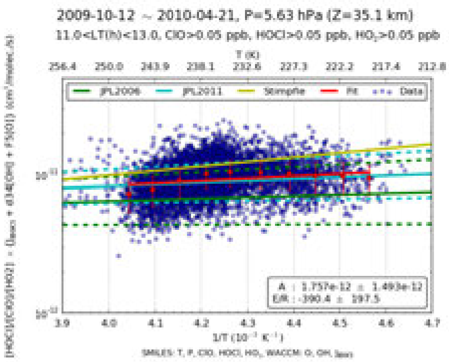
Diurnal variation of ClO, HO_2, and HOCl

Trial to verify the reaction rate of ClO +HO2 using SMILES data









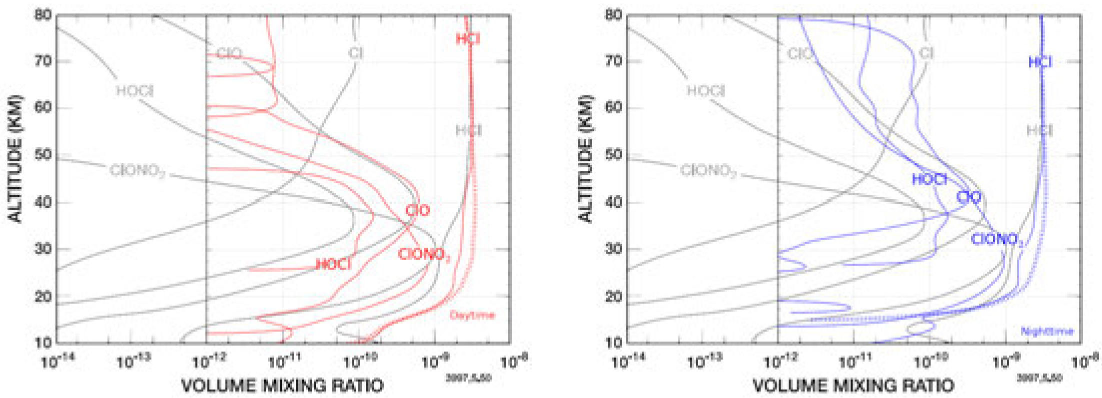
$$ClO + HO_2 \xrightarrow{k_1} HOCl + O_2 \quad (1)$$
$$HOCl + OH \xrightarrow{k_2} H_2O + ClO \quad (2)$$
$$HOCl + h\nu \xrightarrow{j_3} OH + Cl \quad (3)$$

$$O + HOCl \rightarrow OH + ClO \quad (4)$$
$$OH + Cl_2 \rightarrow HOCl + Cl \quad (5)$$
$$OH + OClO \rightarrow HOCl + O_2 \quad (6)$$
$$OH + Cl_2O \rightarrow HOCl + ClO \quad (7)$$
$$OH + Cl_2O_2 \rightarrow HOCl + ClOO \quad (8)$$
$$OH + ClNO_2 \rightarrow HOCl + NO_2 \quad (9)$$
$$Cl + HOCl \rightarrow \text{products} \quad (10)$$

$$k_1 = \frac{[HOCl]}{[HO_2][ClO]}(j_3 + k_2[OH] + k_4[O])$$

Chlorine partitioning in the middle atmosphere

Daytime profiles **Nighttime profiles**



Brasseur and Solomon, pp.373

SMILES (+ MIPAS) can provide knowledge of chlorine partitioning in the background atmosphere based upon observations. The above figures are based on observations on October 12, 2009 at local solar noon (53N-60N) and midnight (23S-33S). ClONO2 is taken from MIPAS IMK, day 51N-57N, night 50N-54N.

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Validation of HCl data from the Superconducting Submillimeter-Wave Limb-Emission Sounder (SMILES)

by Shiotani et al.

(in preparation)

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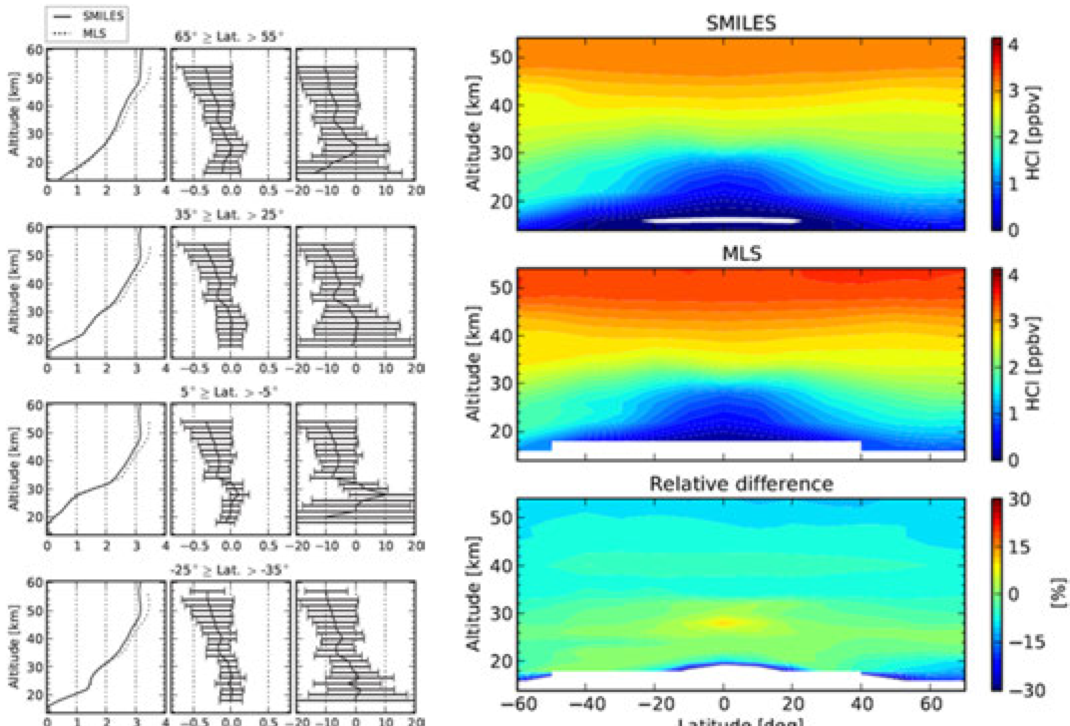
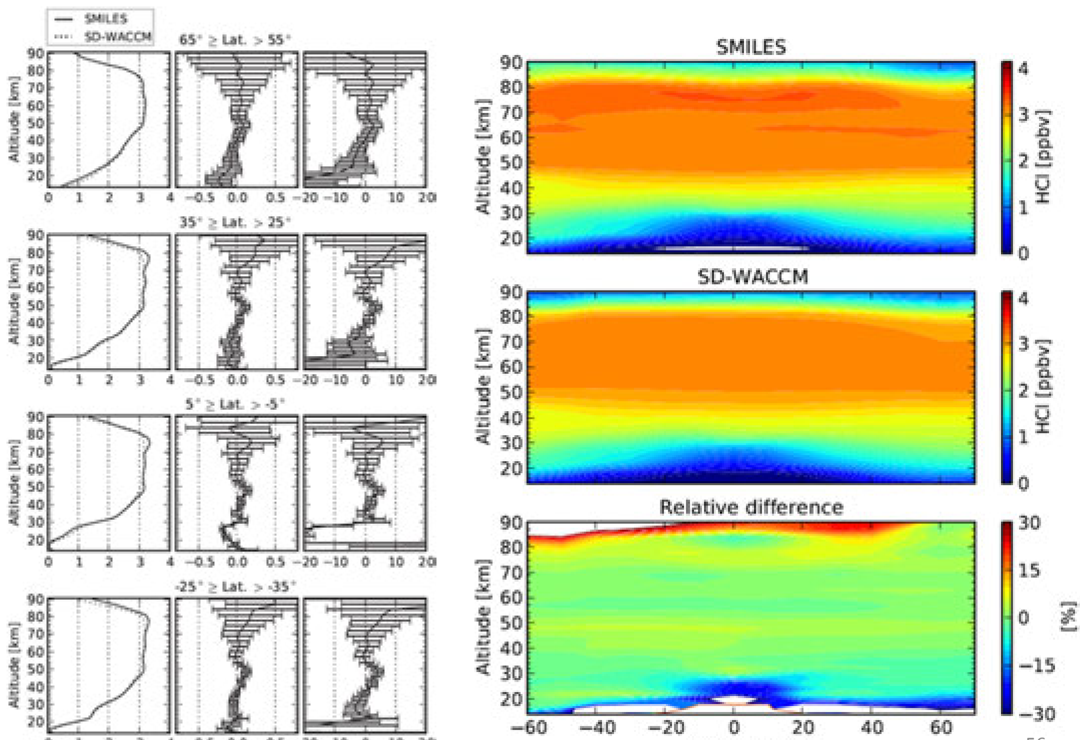
SMILES and MLS comparisons



55

SMILES and SD-WACCM comparisons



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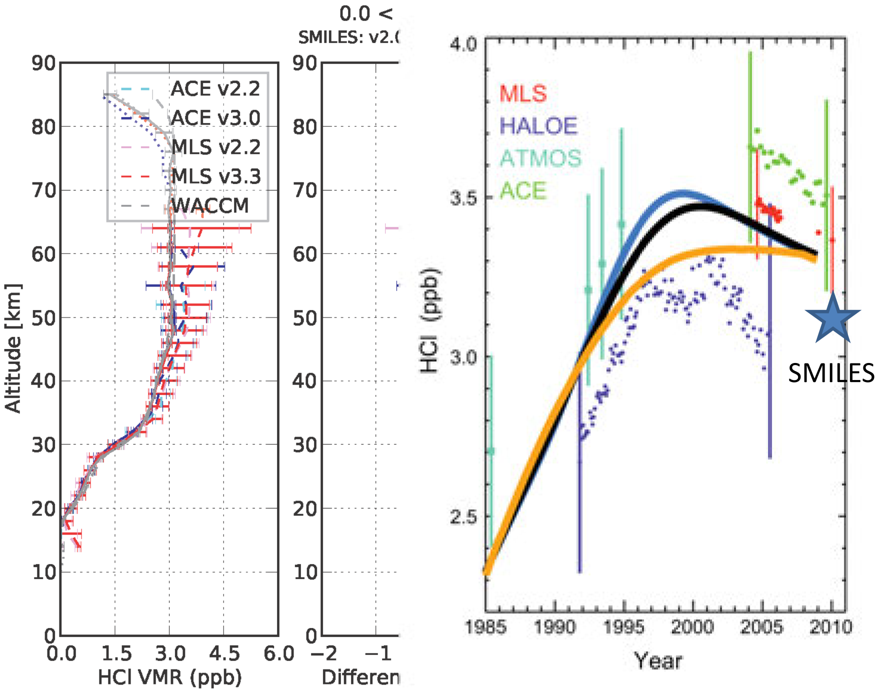
HCl in the middle atmosphere

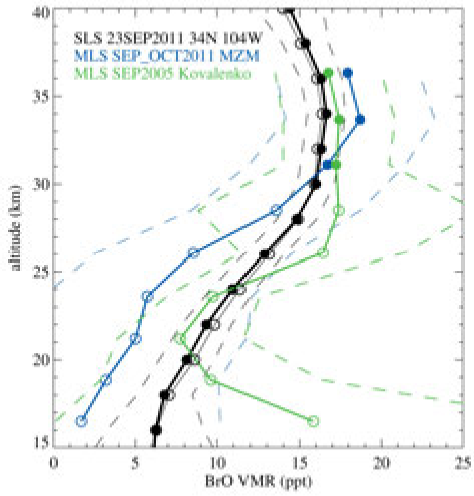


Stratospheric BrO abundance measured by a balloon-borne submillimeterwave radiometer

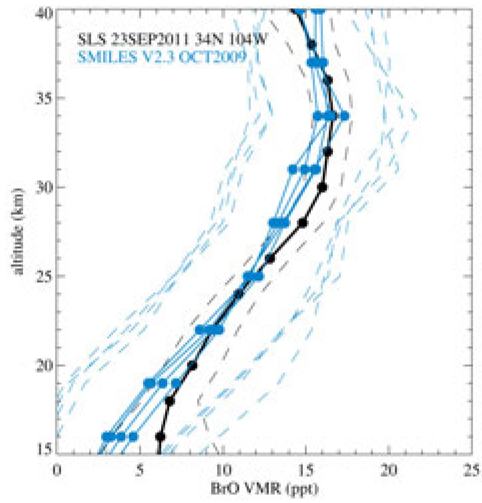
by Stachnik et al.
(accepted, ACP)

BrO observations

MLS



SMILES



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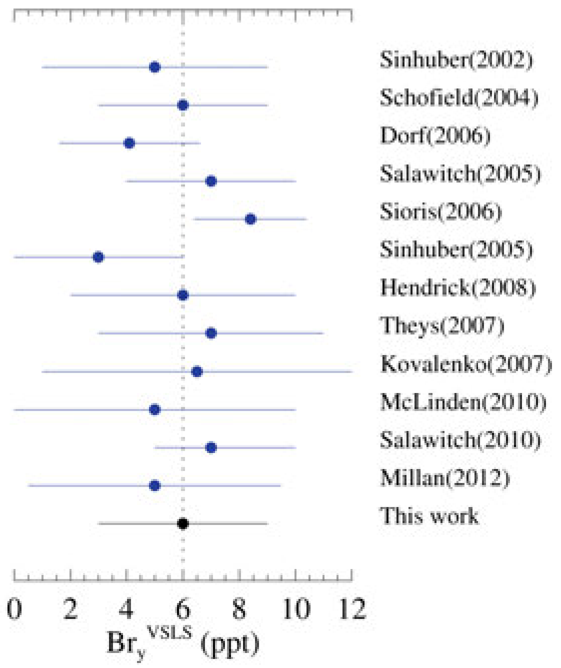
estimations of the VSLS contribution to stratospheric inorganic bromine



60

SMILES Ice Cloud products

by Millan et al.
(accepted, JGR)

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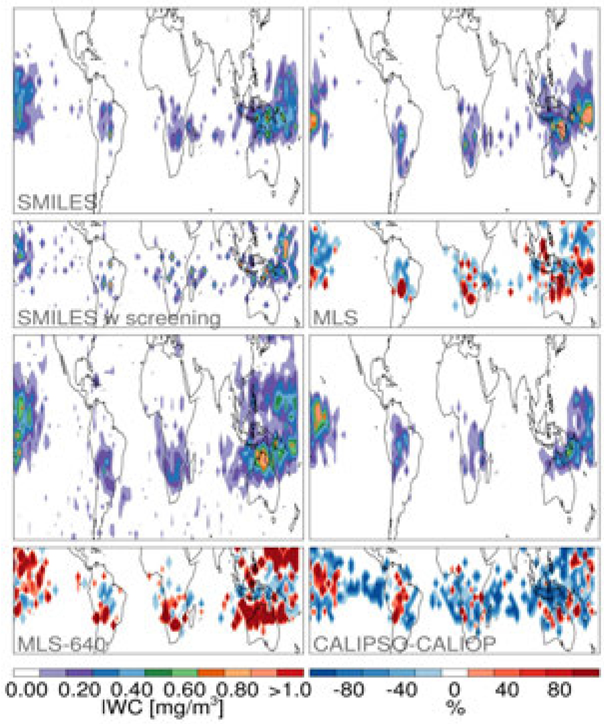
Ice water content for January 2010



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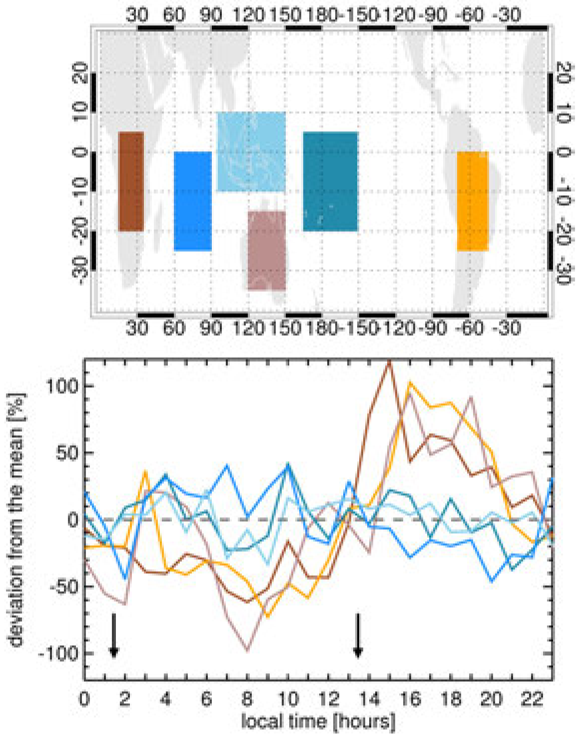
Diurnal variation in pIWP (partial Ice Water Path)



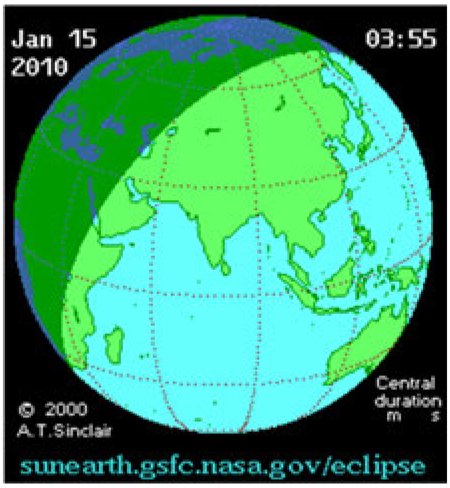
63

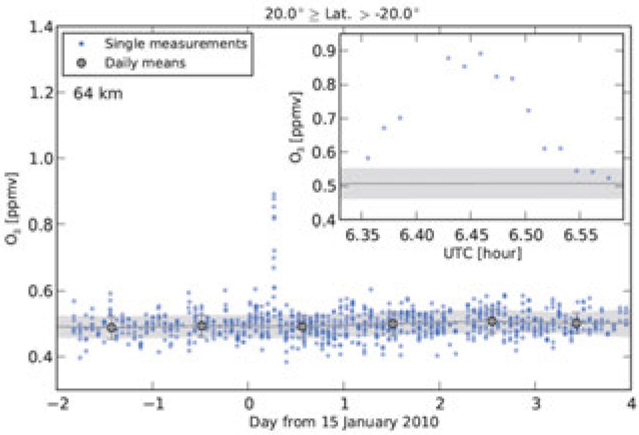
Atmospheric Response During Annular Solar Eclipse on 15 January 2010

by Imai et al.
(will be presented at AOGS 2013)

64

Solar eclipse on January 15, 2010





Night-time O_3 is ~1.2 ppmv at 64km

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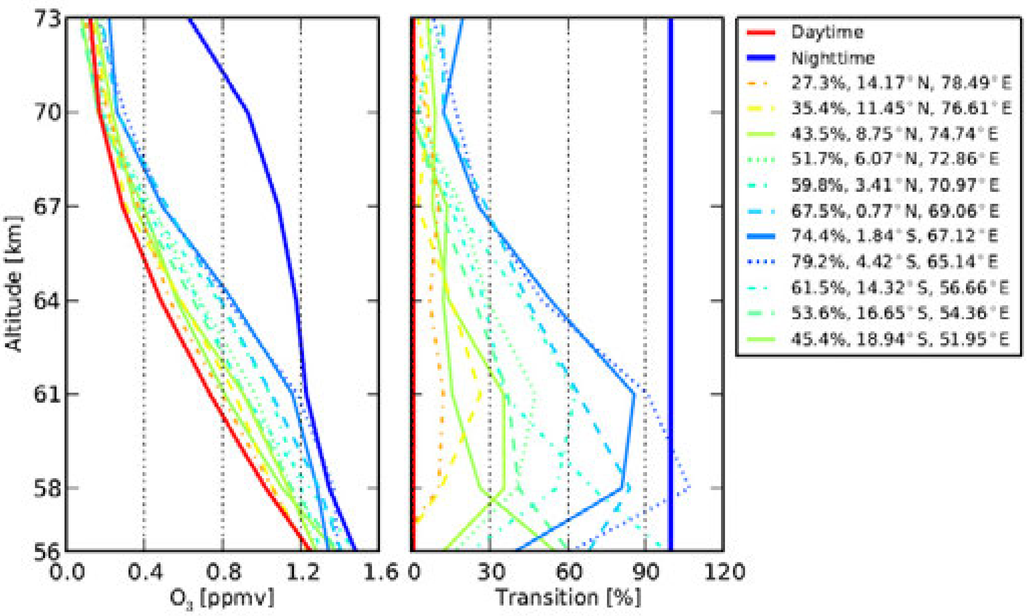
SMILES measurements for ozone



66

SUMMARY

- SMILES made high sensitivity measurements with lower noise than other instruments, and reasonable retrieval results are coming out.
- Diurnal variation of such as O_3, ClO and so on is one of the unique outcomes contributing to scientific issues in the middle atmosphere.
- We released the SMILES level 2 data to the science community in March 2012.

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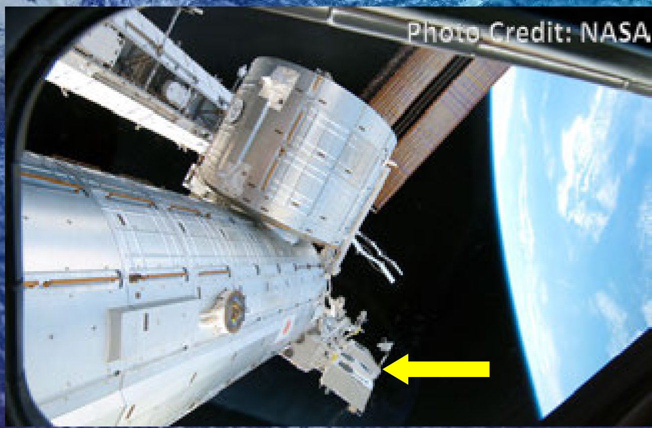
Instrument Development and Onboard Operation

T. Nishibori, S. Mizobuchi (JAXA)



28-29 Mar 2013, SMILES Science evaluation panel 1

Scope of This Presentation

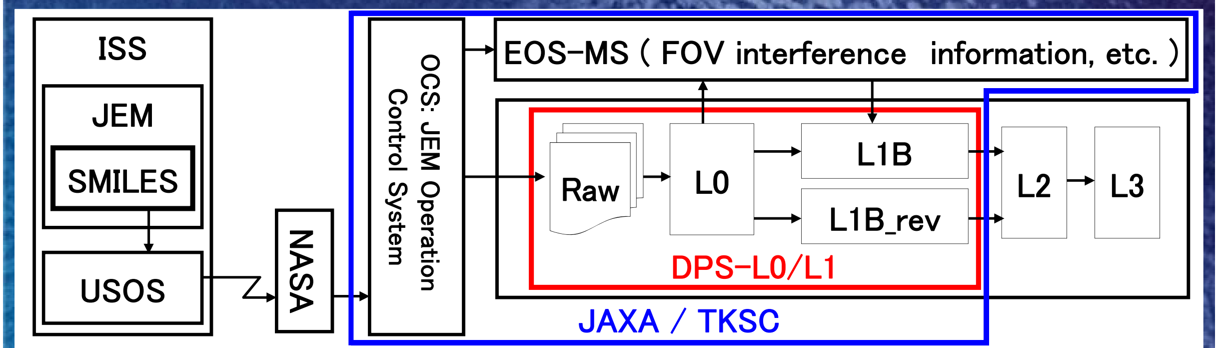
- Data Processing System (DPS-L0/L1) is shortly introduced and its development history are shown.
- Operation and instrument status during the scientific operation phase are briefly presented.
- Overall performance and data quality during the scientific observation phase are evaluated.
- It may not helpful for scientific analysis so much, but will help to understand SMILES.

28-29 Mar 2013, SMILES Science evaluation panel 2

LEVEL1 PROCESSING SYSTEM

Ref. : S. Ochiai et al., "Superconducting Submillimeter-Wave Limb-Emission Sounder on the International Space Station I: Radiometric and spectral calibration and data processing," Journal of the National Institute of Information and Communications Technology, vol. 55, no. 1, pp. 83–95, 2008. [Online]. Available: http://www.nict.go.jp/publication/shuppan/kihou-journal/journal-vol55no1/07-02.pdf

Data Flow

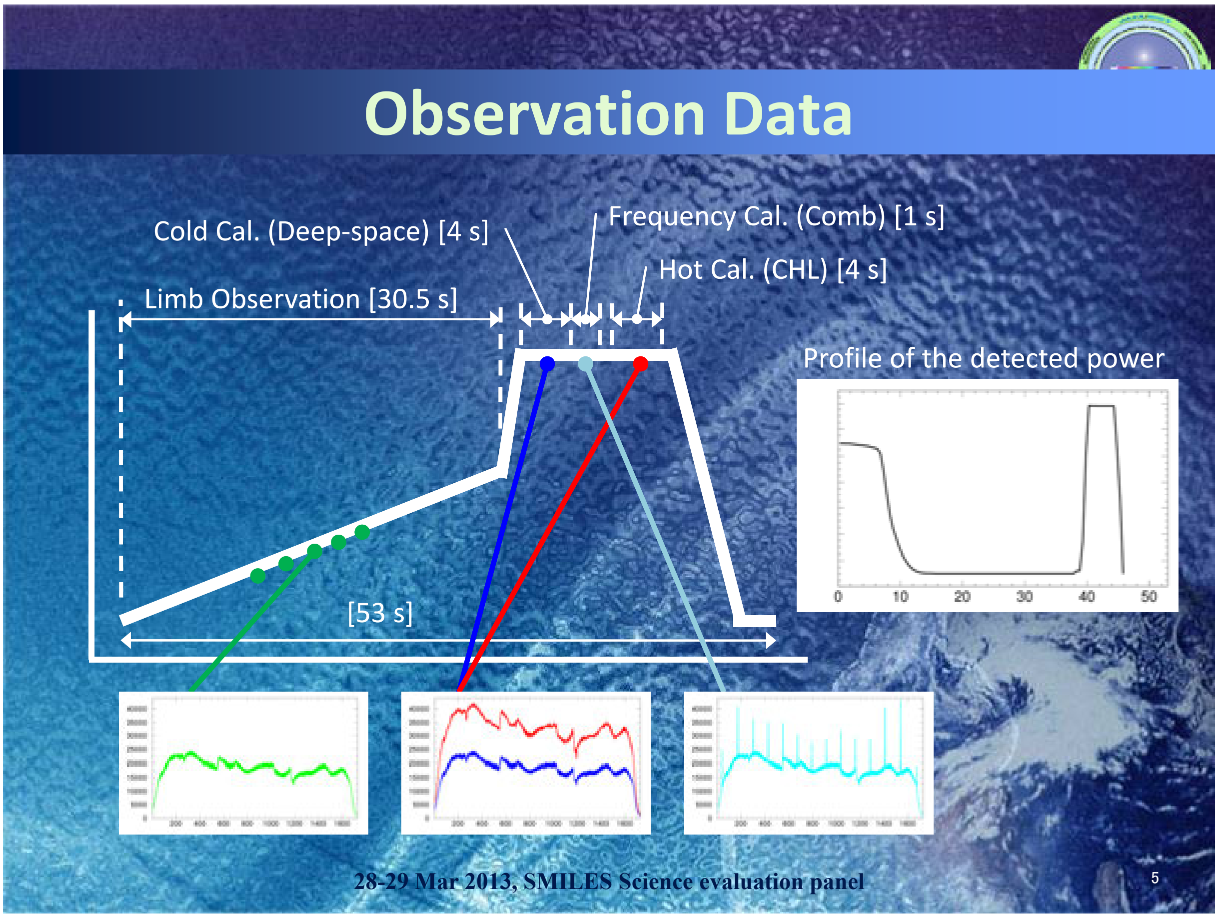


Level 0 [L0] (= Mission Data)

- Raw binary data constructed by SMILES on-board computer every 53 s. (DPS-L0/L1 reconstructs it from the down-linked packets.)
- Including AOS outputs, star tracker outputs, all house-keeping data and so on.

Level 1B [L1B/L1B_rev]

- Calibrated limb emission spectra. Including the spectra , tangent points, calibrated frequencies, SZA, Doppler speed, flags and so on.


Observation Data
Cold Cal. (Deep-space) [4 s]
Frequency Cal. (Comb) [1 s]
Hot Cal. (CHL) [4 s]
Limb Observation [30.5 s]
Profile of the detected power
[53 s]
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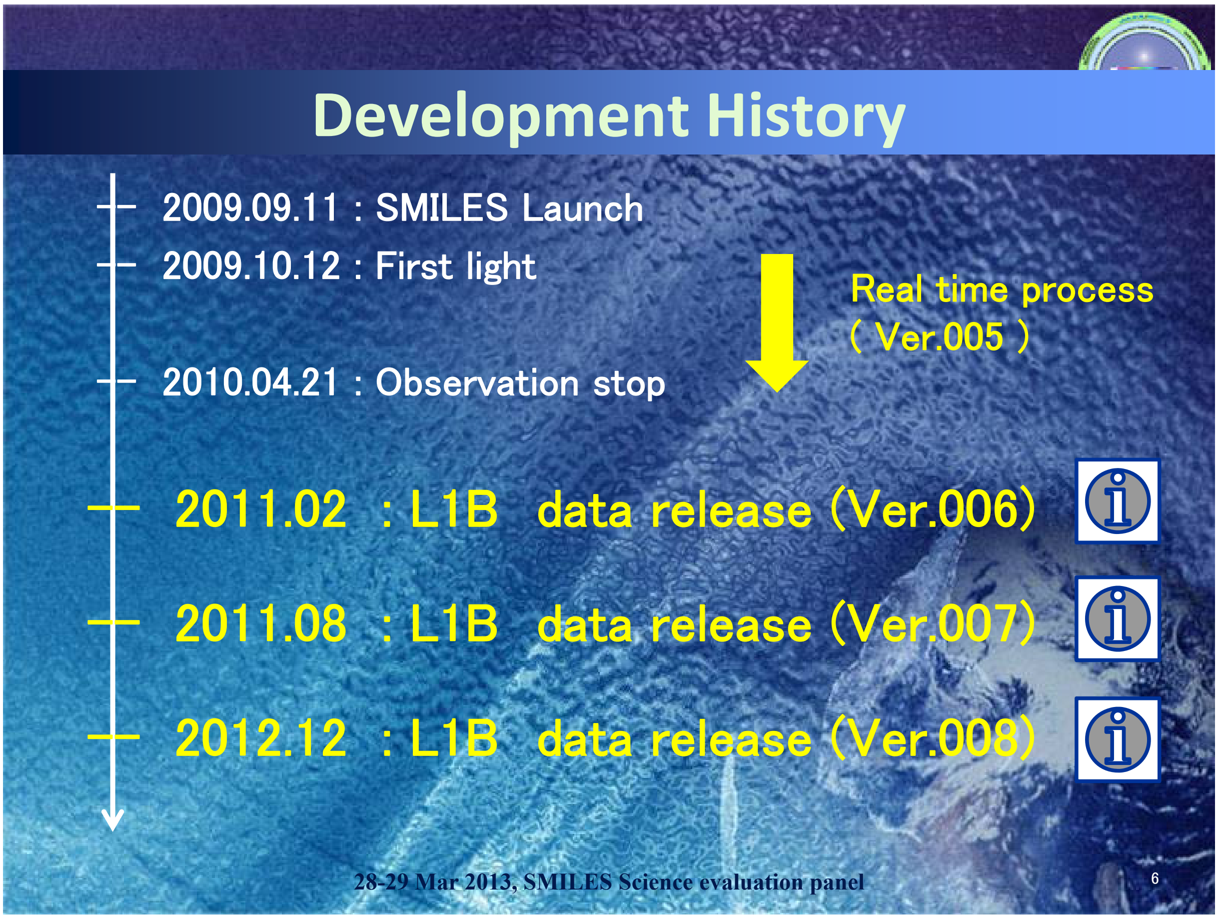
Development History
2009.09.11 : SMILES Launch
2009.10.12 : First light
2010.04.21 : Observation stop
Real time process
(Ver.005)
2011.02 : L1B data release (Ver.006)
2011.08 : L1B data release (Ver.007)
2012.12 : L1B data release (Ver.008)
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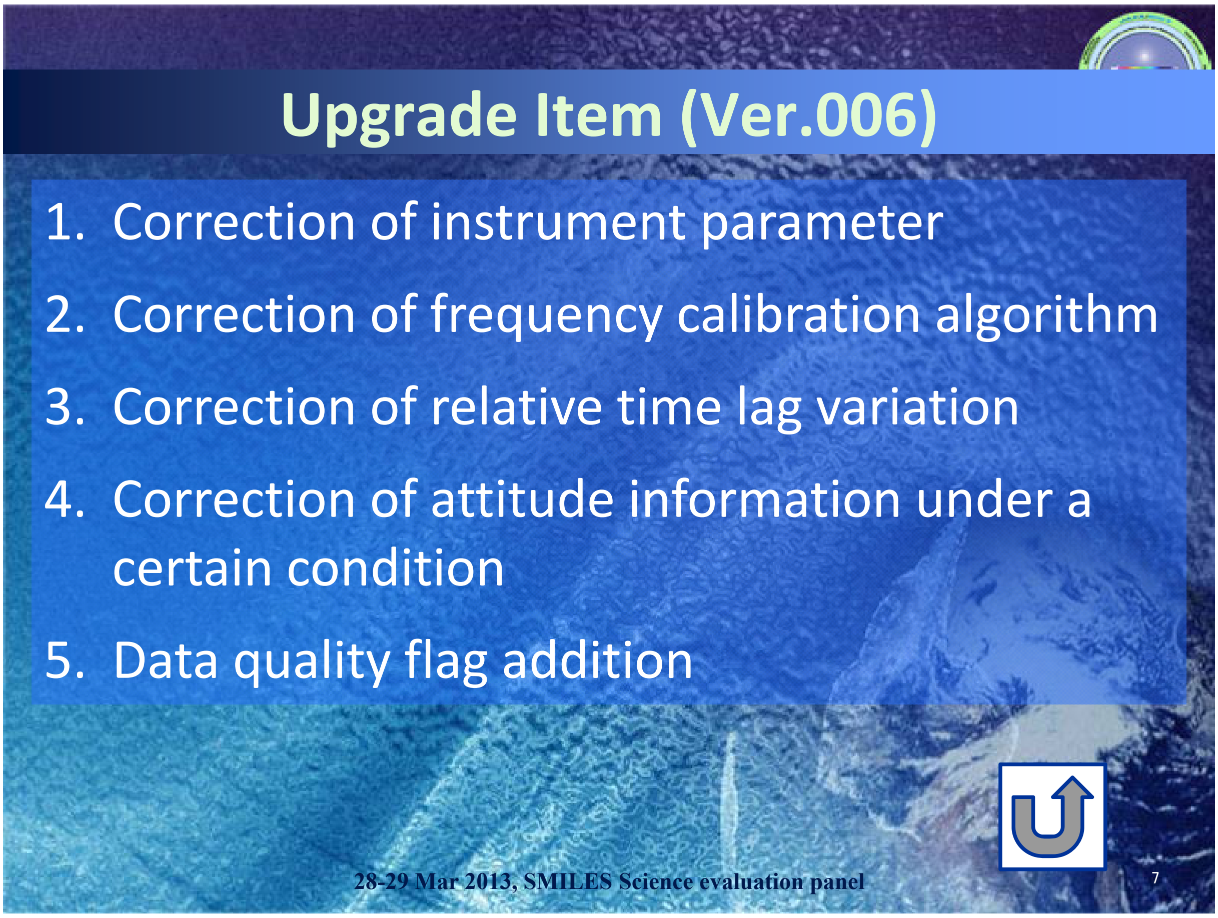
Upgrade Item (Ver.006)
1. Correction of instrument parameter
2. Correction of frequency calibration algorithm
3. Correction of relative time lag variation
4. Correction of attitude information under a certain condition
5. Data quality flag addition
28-29 Mar 2013, SMILES Science evaluation panel
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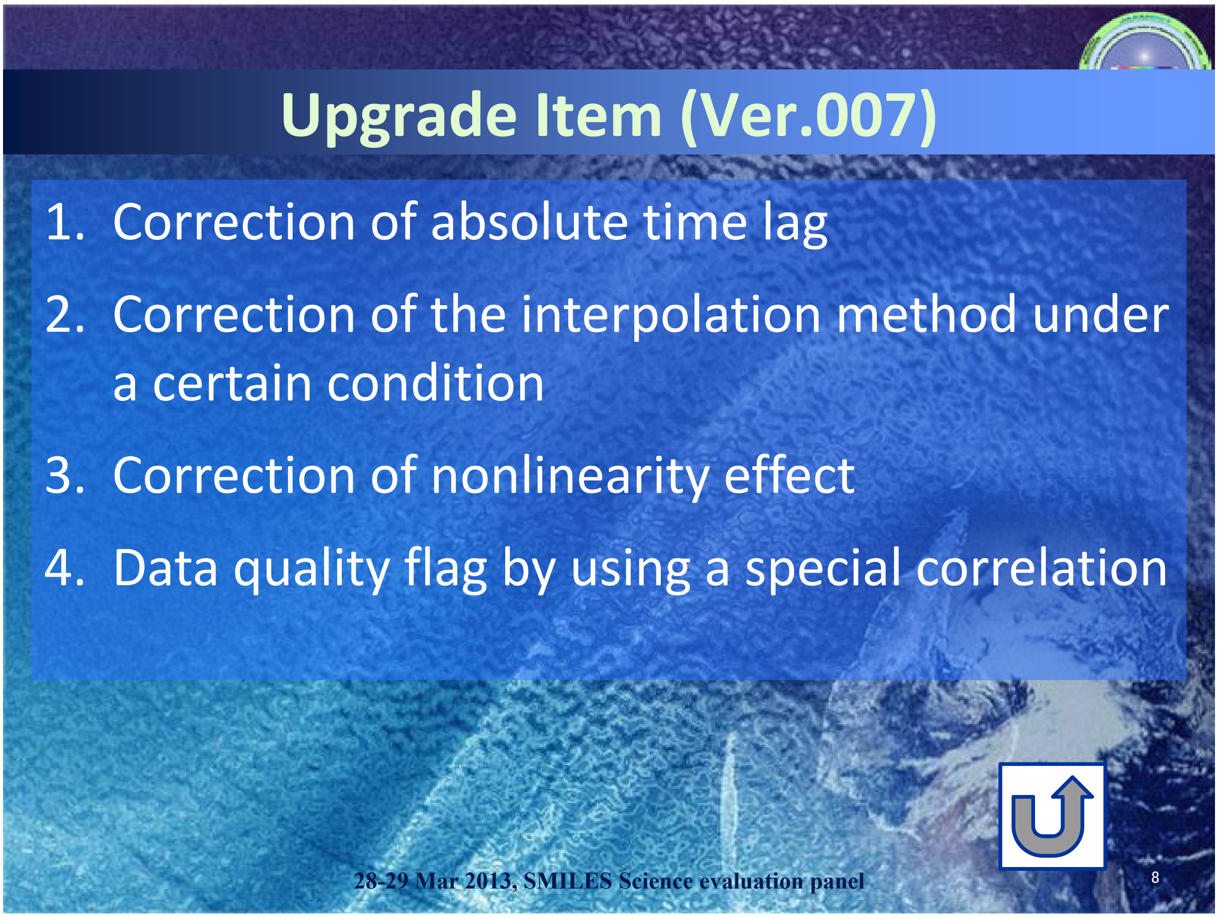
Upgrade Item (Ver.007)
1. Correction of absolute time lag
2. Correction of the interpolation method under a certain condition
3. Correction of nonlinearity effect
4. Data quality flag by using a special correlation
28-29 Mar 2013, SMILES Science evaluation panel
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Upgrade Item (Ver.008)

1. A smoothing treatment of the altitude data
2. Data quality flag by using a instrument status parameter
3. Correction of frequency calibration algorithm
4. Recalibration of the instrument parameters
5. Correction of the interpolation method under a certain condition
6. Correction of nonlinearity effect

OPERATION STATISTICS


Operation History
2009
2010
Aug
Sep
Oct
Nov
Dec
Jan
Feb
Mar
Apr
May
Jun
Jul
Aug
Sep
Launch
Initial C/O
Normal Operation
Local Oscillator Trouble
Cryocooler Trouble
Scientific Operation
(L0/L1b)
12 Oct 2009
21 Apr 2010
28-29 Mar 2013, SMILES Science evaluation panel
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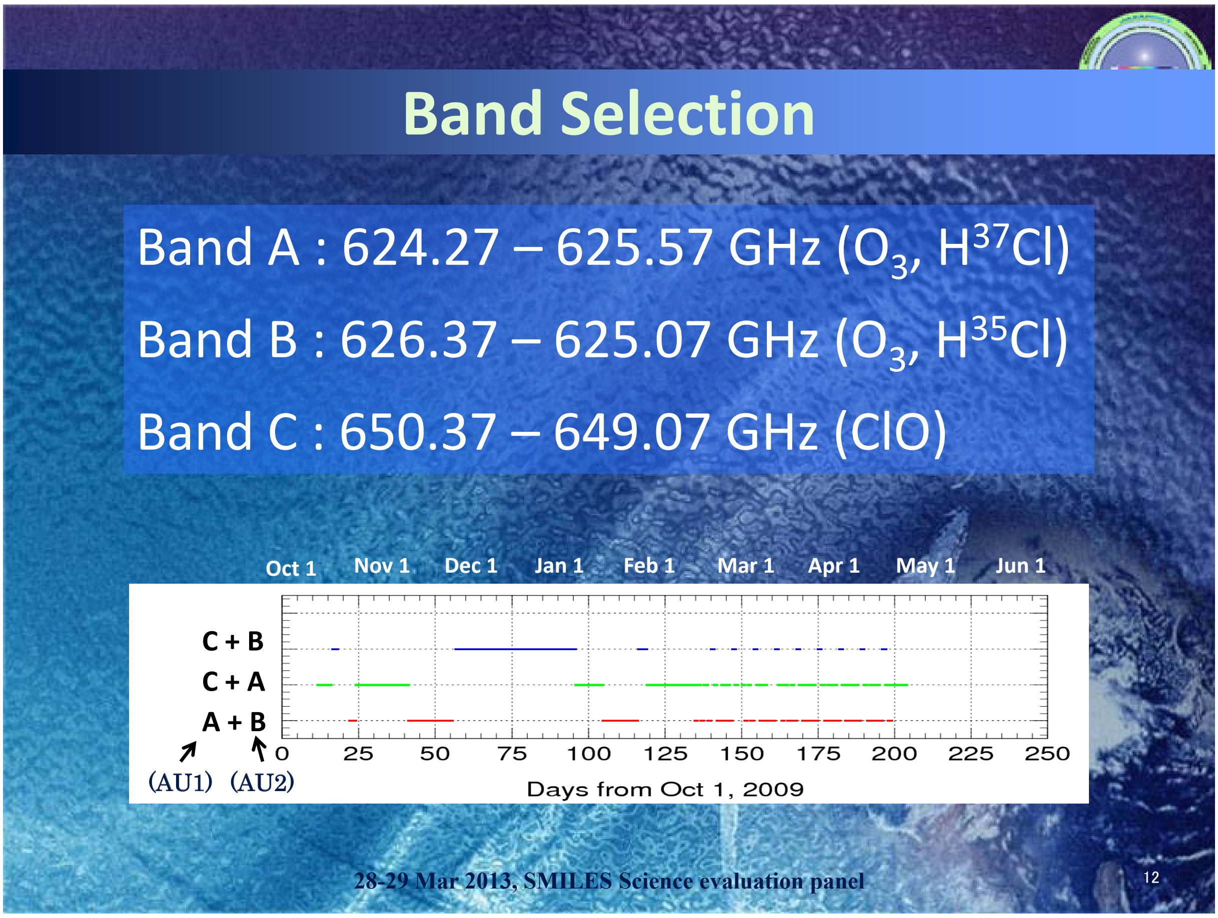
Band Selection
Band A : 624.27 – 625.57 GHz (O3, H37Cl)
Band B : 626.37 – 625.07 GHz (O3, H35Cl)
Band C : 650.37 – 649.07 GHz (ClO)
Oct 1
Nov 1
Dec 1
Jan 1
Feb 1
Mar 1
Apr 1
May 1
Jun 1
C + B
C + A
A + B
0
25
50
75
100
125
150
175
200
225
250
Days from Oct 1, 2009
(AU1)
(AU2)
28-29 Mar 2013, SMILES Science evaluation panel
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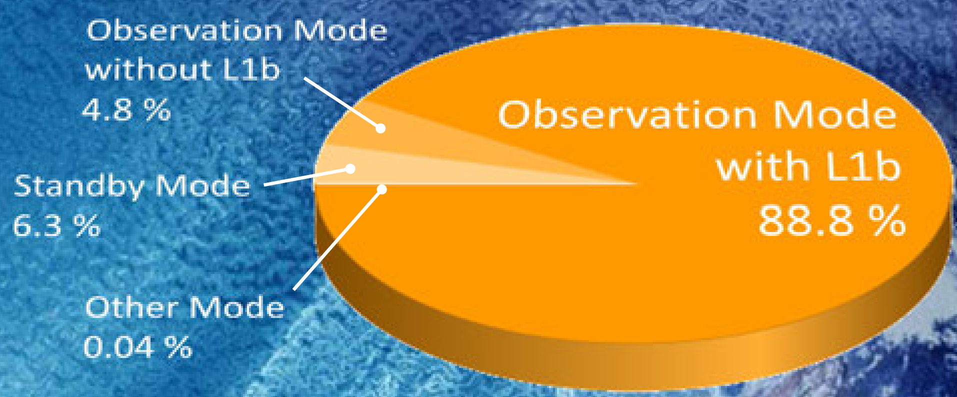
L0/L1b Yield (1/2)

- Period:
  12-Oct-2009 ~ 21-Apr-2010 (total 191 days)



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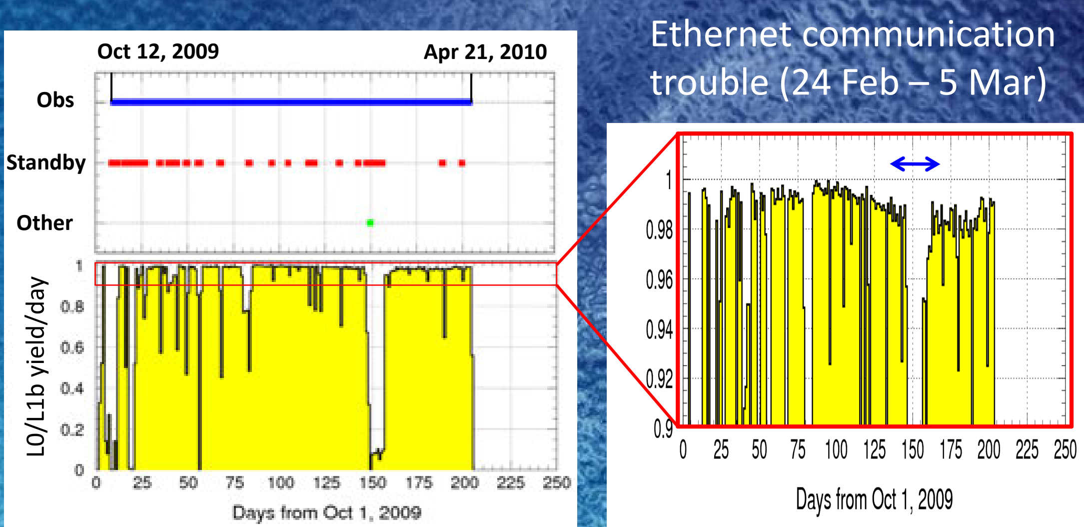
L0/L1b Yield (2/2)



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"Available" Data

- Total 276,990 L1b (ver. 008) data are available in the operation period (12-Oct-2009 ~ 21-Apr-2010).
- The number of L1b data may be much lower for atmospheric analysis.
  - No FOV interference
  - Proper tangent height
  - …

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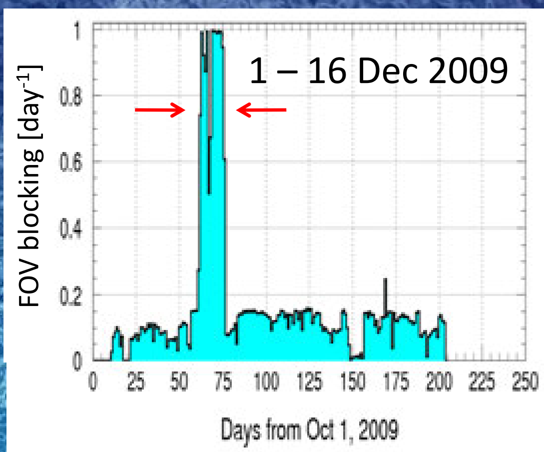
FOV Interference

- ISS's solar paddle across the FOV cases ~10 % loss in every orbit



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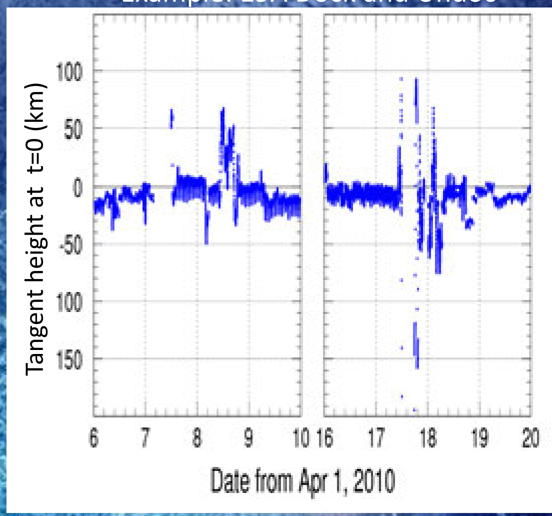
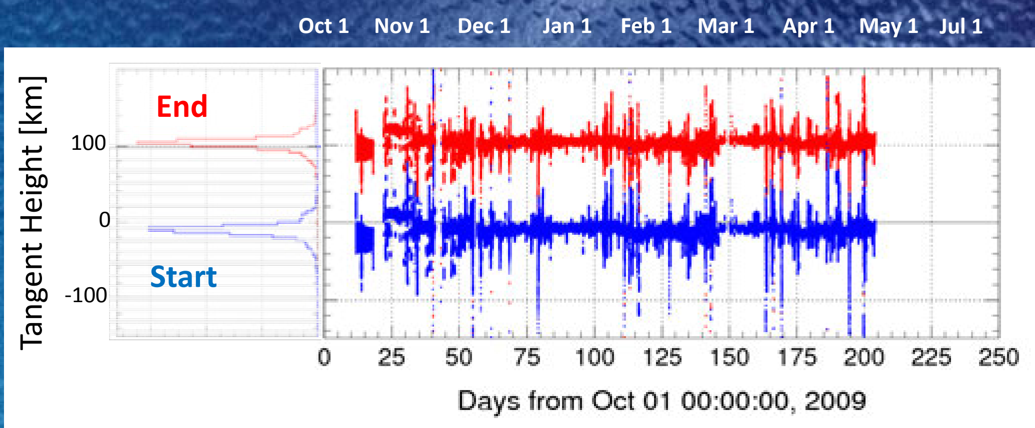
Attitude Variation due to Dock and Undock Events

Date	Vehicle	Event
2009/10/11 01:07	18S	Undock
2009/10/18 01:40	35P	Dock
2009/10/30 17:32	HTV1	Undock
2009/11/12 15:41	5R	Dock
2009/11/16 19:28	ULF3	Dock
2009/11/25 09:53	ULF3	Undock
2009/12/01 03:34	19S	Undock
2009/12/22 22:48	21S	Dock
2010/02/05 04:25	36P	Dock
2010/02/09 17:06	20A	Dock
2010/02/20 00:54	20A	Undock
2010/03/18 08:03	20S	Undock
2010/04/04 05:25	22S	Dock
2010/04/07 07:44	19A	Dock
2010/04/17 12:52	19A	Undock

Example: 19A Dock and Undoc



Tangent Height Variation



Scan period	Mean [km]	Sigma [km]
End of Scan (t=30s)	103.17	12.32
Start of Scan (t=0s)	-10.27	13.99

INSTRUMENT STATUS

28-29 Mar 2013, SMILES Science evaluation panel

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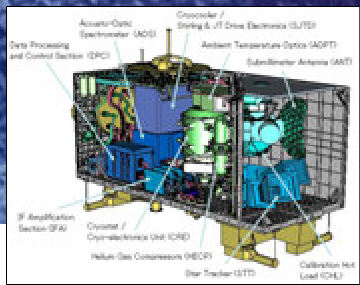
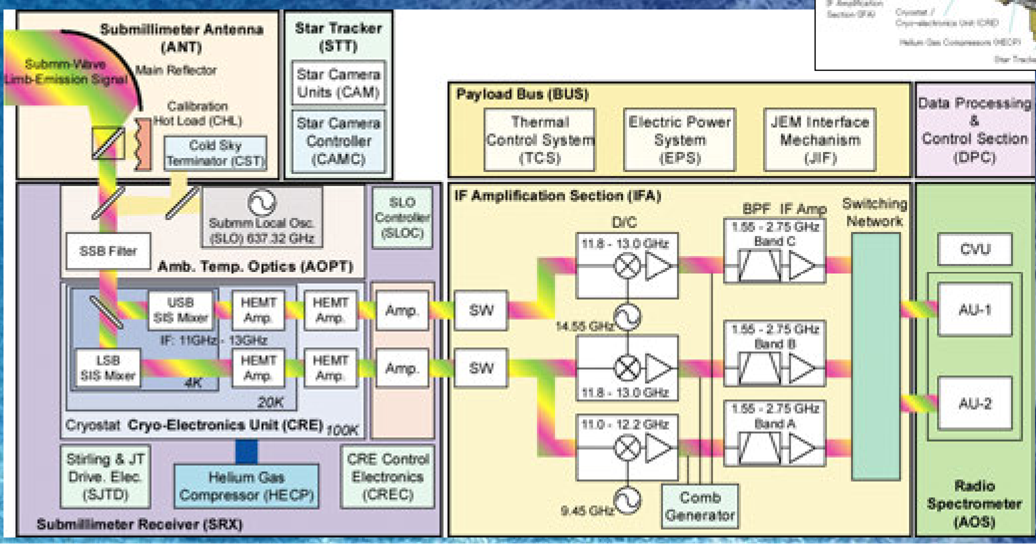
Instrument Block Diagram

- ANT SRX IFA AOS
- STT BUS DPC





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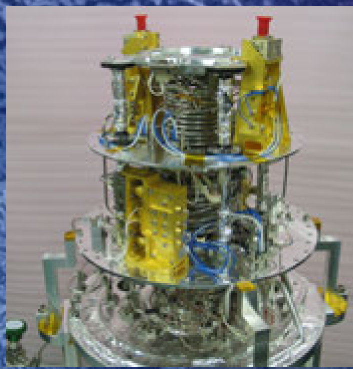
Mechanical Cooler and SIS Mixer

- Mechanical Cooler
  - Two-stage stirling and J-T
  - Cooling Capacity :
    20mW @ 4K, 200mW @ 20K,
    1000mW @ 100K
  - Power Consumption : < 300 W
  - Mass : 90 kg
- SIS Mixer
  - RF : 640 GHz
  - IF : 11-13 GHz
  - Junction : Nb/AlOx/Nb, ~ 7 kA/cm^2
  - RF Matching : PCTJ with Integrated Circuit
  - Fabricated at Nobeyama RO



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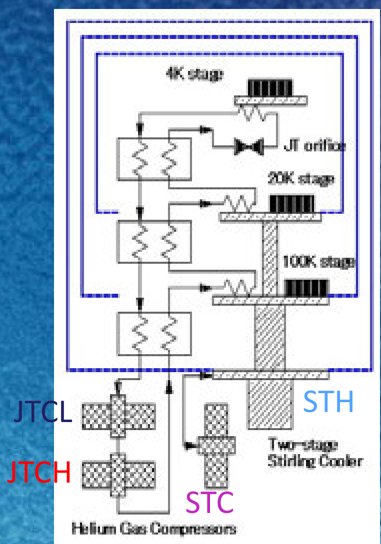
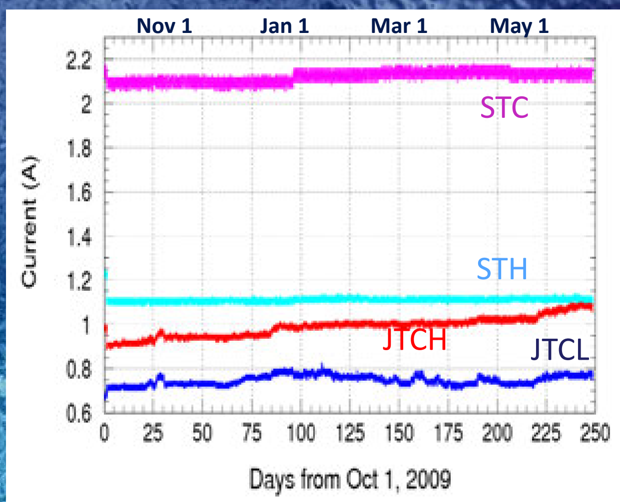
Compressor Performance





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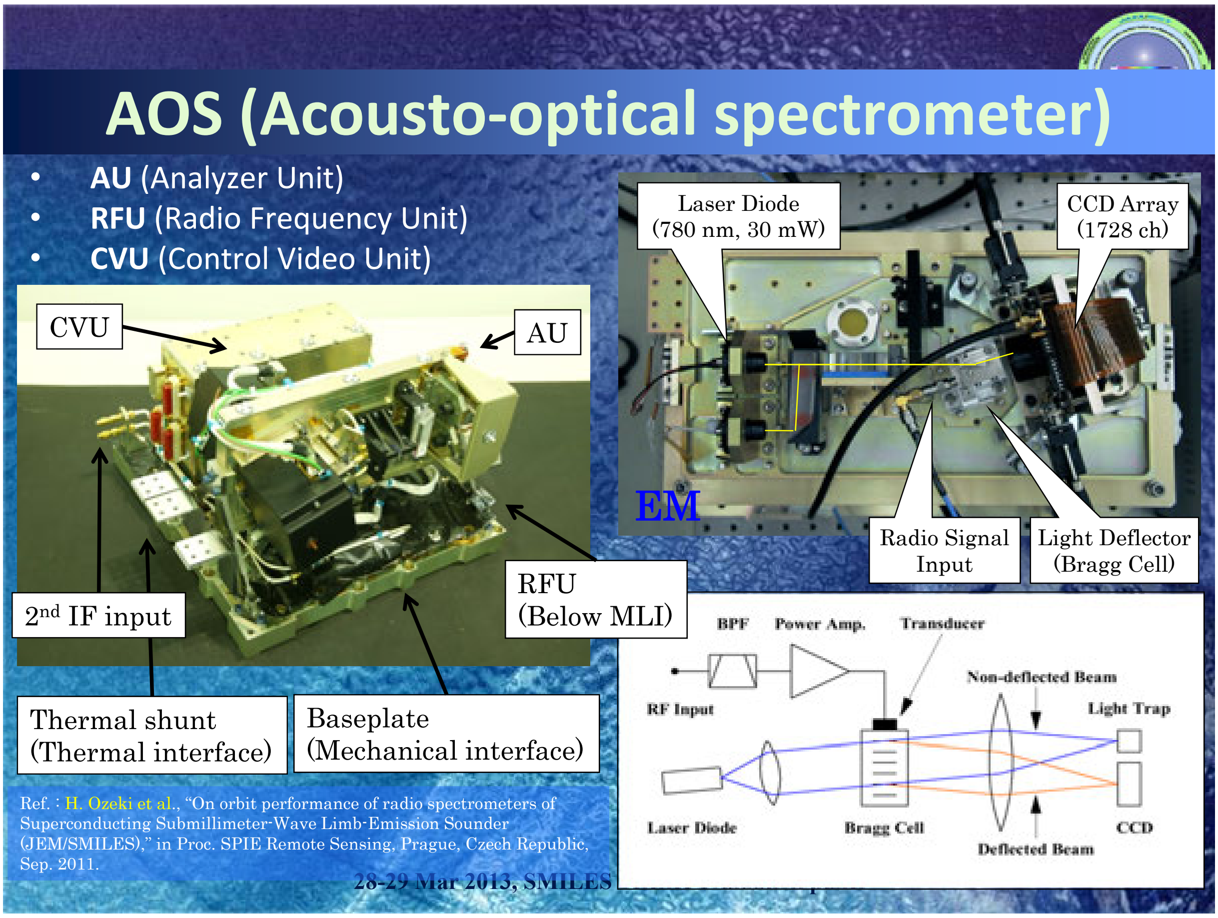
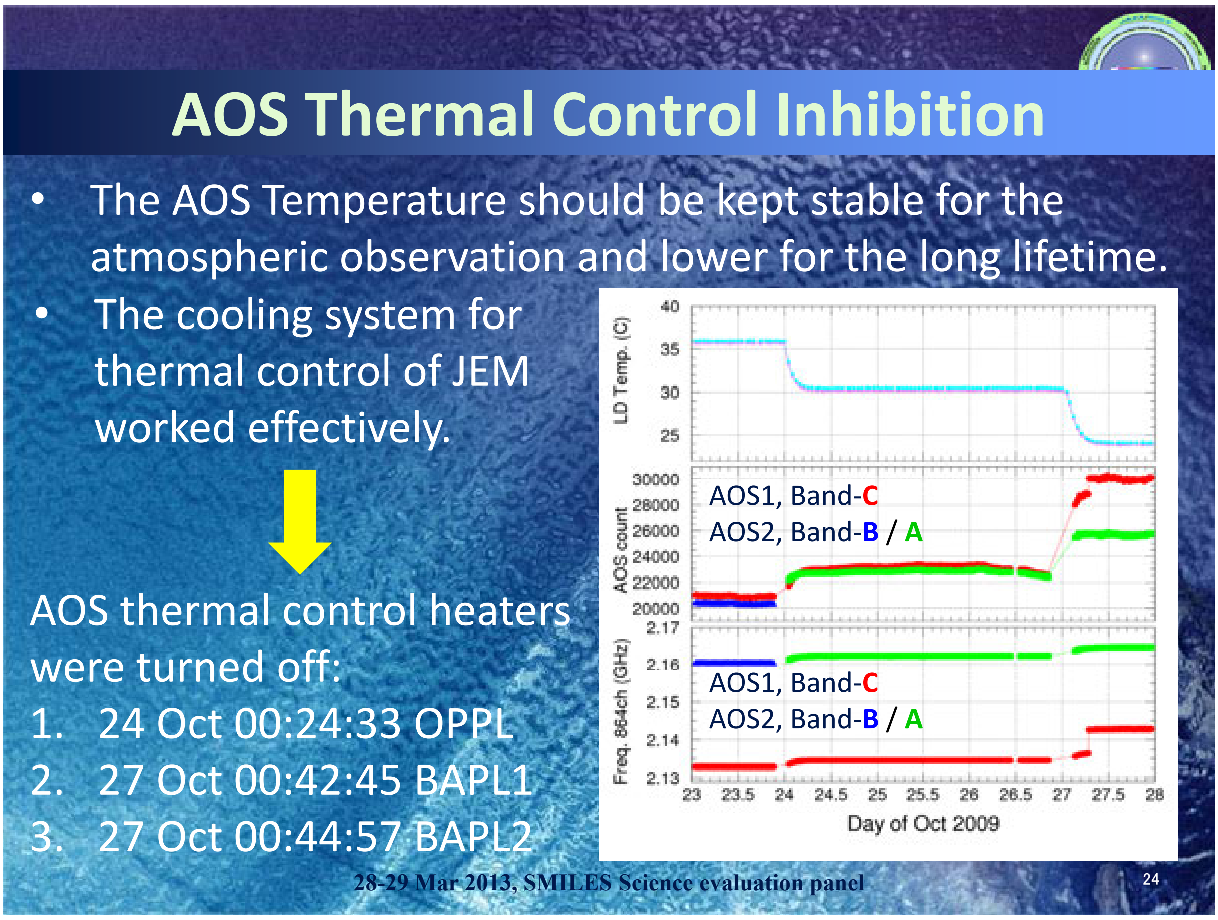

AOS (Acousto-optical spectrometer)
• AU (Analyzer Unit)
• RFU (Radio Frequency Unit)
• CVU (Control Video Unit)
CVU
AU
2nd IF input
RFU (Below MLI)
Thermal shunt (Thermal interface)
Baseplate (Mechanical interface)
Laser Diode (780 nm, 30 mW)
CCD Array (1728 ch)
EM
Radio Signal Input
Light Deflector (Bragg Cell)
BPF
Power Amp.
Transducer
Non-deflected Beam
RF Input
Light Trap
Laser Diode
Bragg Cell
CCD
Deflected Beam
Ref. : H. Ozeki et al., "On orbit performance of radio spectrometers of Superconducting Submillimeter-Wave Limb-Emission Sounder (JEM/SMILES)," in Proc. SPIE Remote Sensing, Prague, Czech Republic, Sep. 2011.
28-29 Mar 2013, SMILES


AOS Thermal Control Inhibition
• The AOS Temperature should be kept stable for the atmospheric observation and lower for the long lifetime.
• The cooling system for thermal control of JEM worked effectively.
AOS thermal control heaters were turned off:
1. 24 Oct 00:24:33 OPPL
2. 27 Oct 00:42:45 BAPL1
3. 27 Oct 00:44:57 BAPL2
LD Temp. (C)
AOS count
Freq. 864ch (GHz)
AOS1, Band-C
AOS2, Band-B / A
Day of Oct 2009
28-29 Mar 2013, SMILES Science evaluation panel
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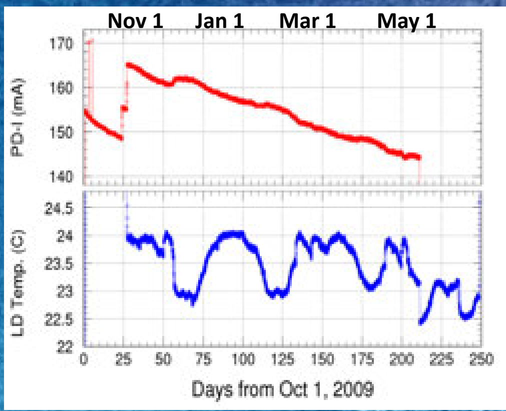
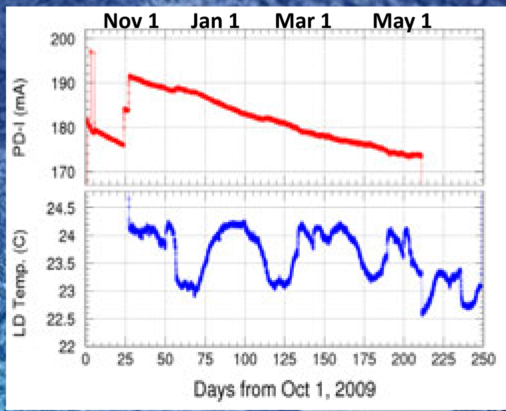
AOS Laser Diode

AOS1



AOS2



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OVERALL PERFORMANCE

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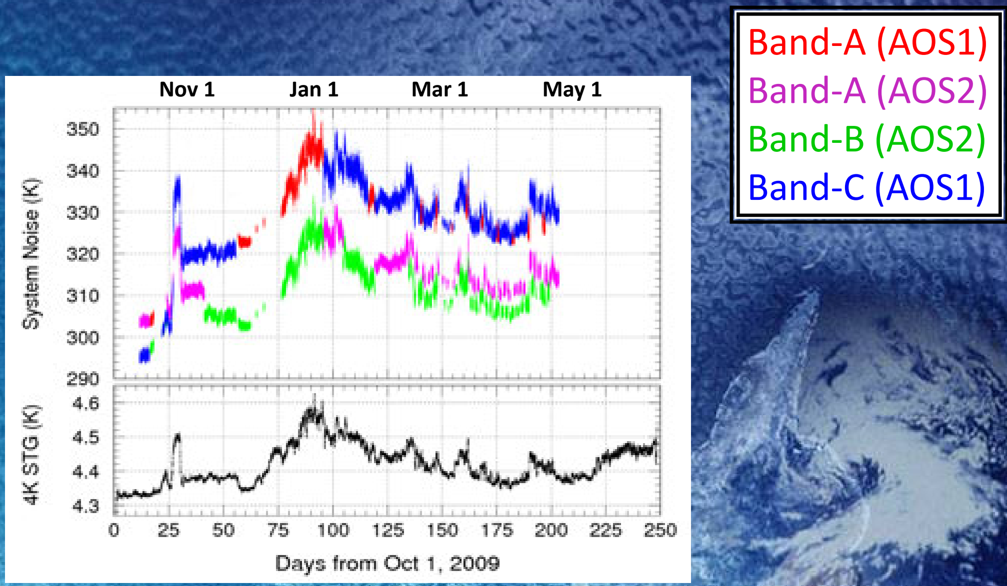
System Noise Temperature



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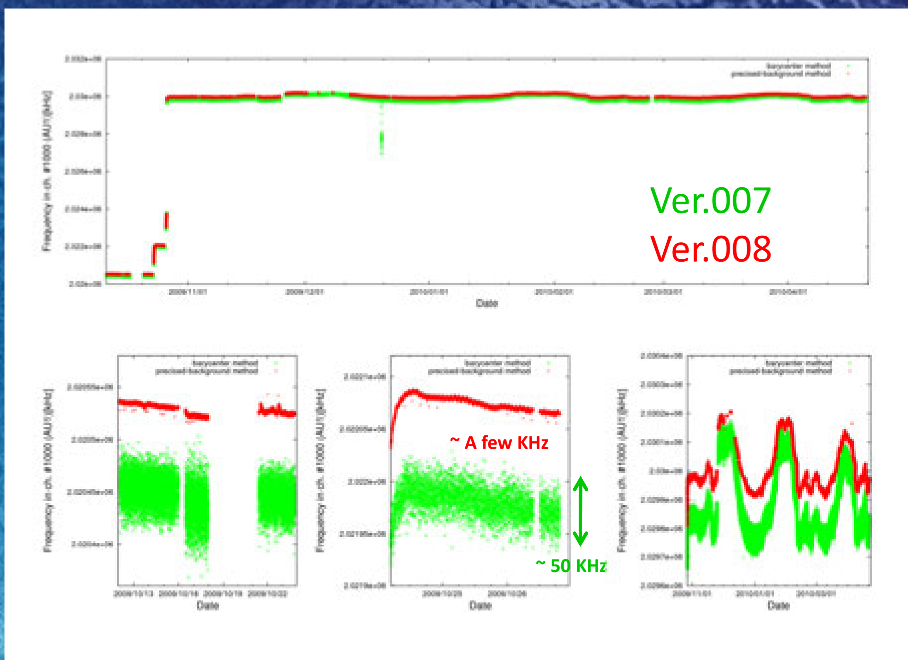
Frequency Calibration (AOS1)



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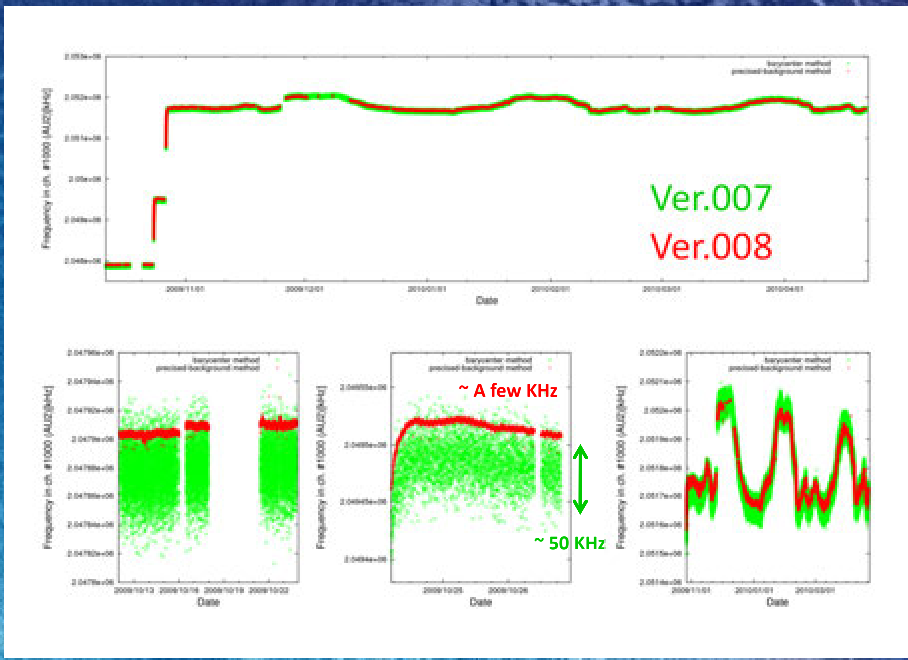
Frequency Calibration (AOS2)



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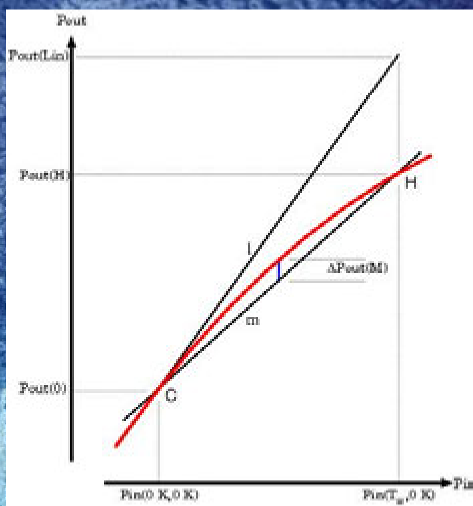
Gain Nonlinearity

- Gain nonlinearity causes a systematic error in the measured atmospheric emission.
- The intensity scaling may have an error of up to 3% by the non-linearity.
- Gain linearity was measured in ground system tests.
- The measured gain linearity was almost consistent with the estimation
- We could know the gain linearity in the accuracy of less than 1%.



Ref. : S. Ochiai et al., "Gain nonlinearity calibration of submillimeter radiometer for JEM/SMILES," IEEE J. Sel. Topics Appl. Earth Obs. Remote Sens., vol. 5, no. 3, pp. 962–969, 2012.

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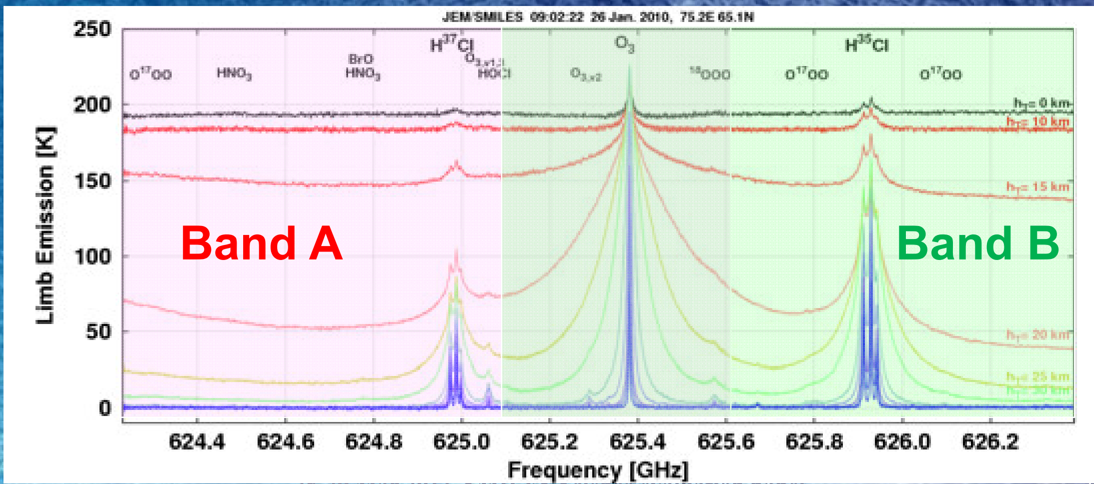
Nonlinearity Correction (1/2)

- SMILES can simultaneously observes ozone line at 625.371 GHz with two receiver backends.
- Observed intensities with two bands must be identical within an error.



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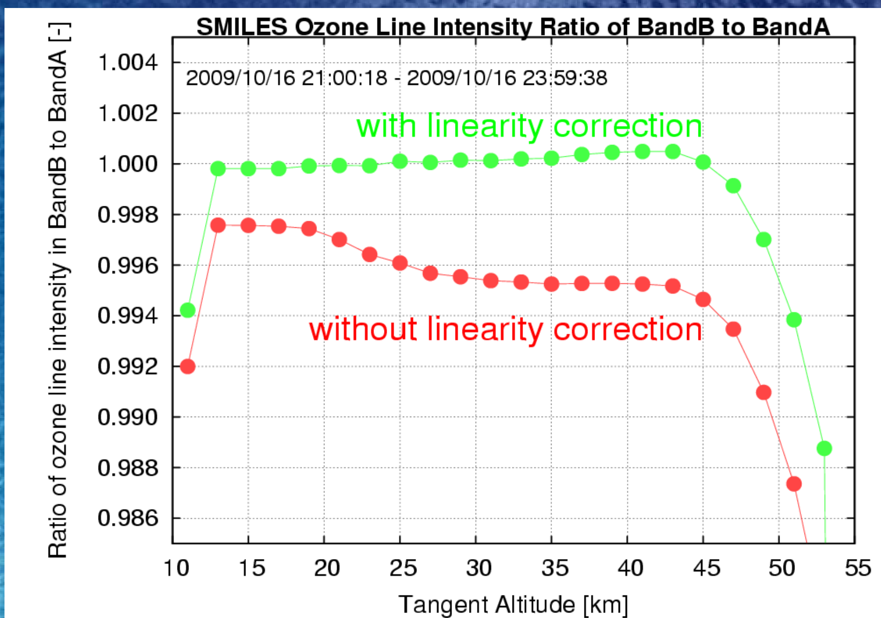
Nonlinearity Correction (2/2)

- Nonlinearity correction improves coincidence.



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DATA QUALITY
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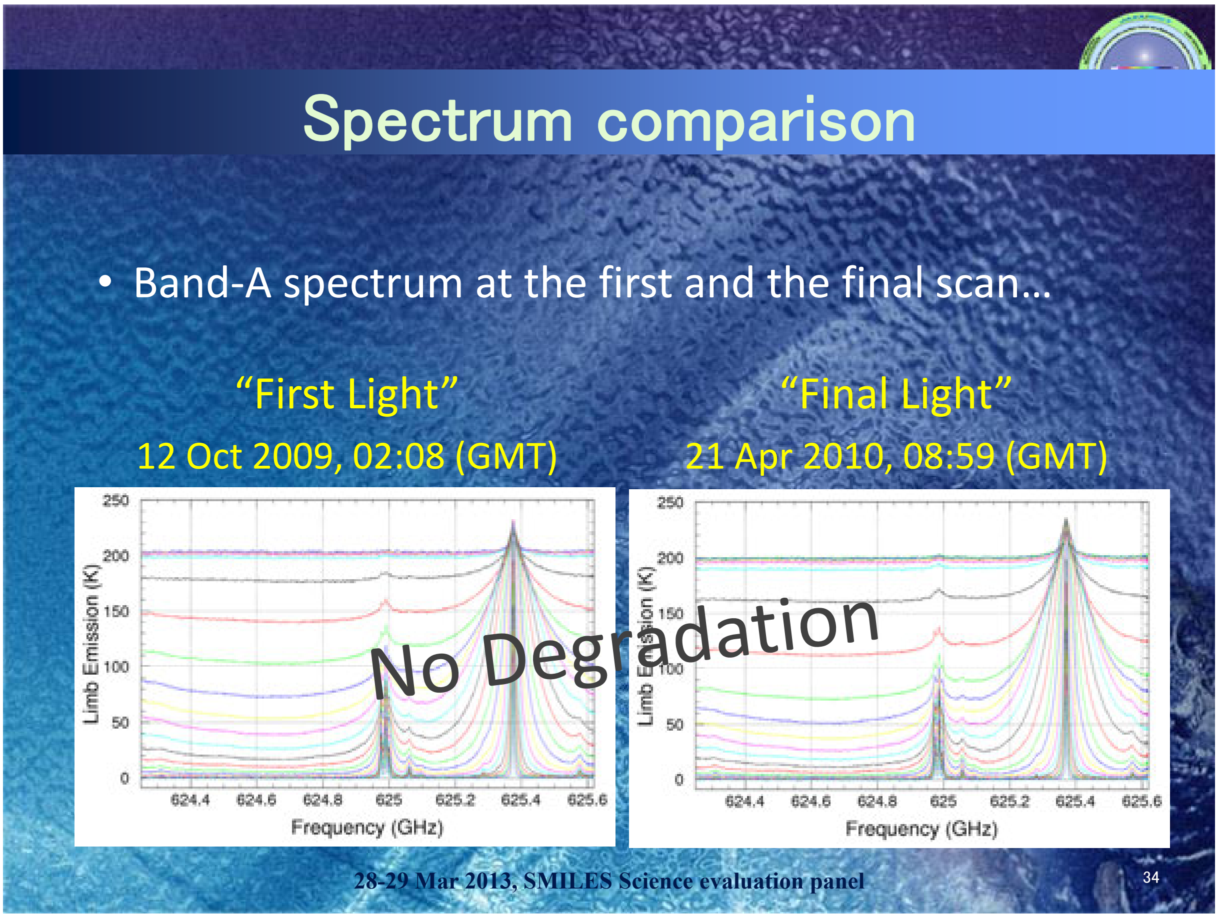
Spectrum comparison
• Band-A spectrum at the first and the final scan...
"First Light"
12 Oct 2009, 02:08 (GMT)
"Final Light"
21 Apr 2010, 08:59 (GMT)
Limb Emission (K)
Frequency (GHz)
No Degradation
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Summary

- Observation data obtained in 12 Oct 2009 – 21 Apr 2010 are available.
- AOS thermal control heaters were turned off in two steps.
- We found deteriorations with age in some instrumental parameters.
  - Decreasing of photo diode current for AOS
  - Increasing of JT compressor driving current
- These deteriorations may not affect L0/L1b data qualities.
- We found no degradation in the data quality throughout the scientific operation period.

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Publication list

K. Kikuchi et al., "Flight model performance of 640-GHz superconductor insulatorsuperconductor mixers for JEM/SMILES mission," J. Infrared, Millimeter, and Terahertz Waves, pp. 1205–1211, 2010.

T. Manabe et al., "Measurement of the offset-Cassegrain antenna of JEM/SMILES using a near-field phase-retrieval method in the 640-GHz band," IEEE Trans. Antennas Propag., vol. 60, no. 8, pp. 3971–3976, 2012.

T. Manabe et al., "Submillimeter-wave antenna and receiver optics for JEM/SMILES," IEICE Transactions on Communications, vol. J95-B, no. 9, pp. 990–1002, 2012 (in Japanese).

S. Mizobuchi et al., "In-orbit measurement of the AOS (acousto-optical spectrometer) response using frequency comb signals," IEEE J. Sel. Topics Appl. Earth Obs. Remote Sens., vol. 5, no. 3, pp. 977–983, 2012.

S. Ochiai et al., "Gain nonlinearity calibration of submillimeter radiometer for JEM/SMILES," IEEE J. Sel. Topics Appl. Earth Obs. Remote Sens., vol. 5, no. 3, pp. 962–969, 2012.

S. Ochiai et al., "Receiver performance of the Superconducting Submillimeter-Wave Limb-Emission Sounder (SMILES) on the International Space Station," Geoscience and Remote Sensing, IEEE Transactions on, vol. 51, no. 7, 2013.

Y. Iida et al., "Space-borne submillimeter wave calibration load with specular absorbers," J. Remote Sensing Society of Japan (in press, in Japanese), vol. 33, no. 2, 2013.

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Thank you !
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Status of SMILES Project in JAXA

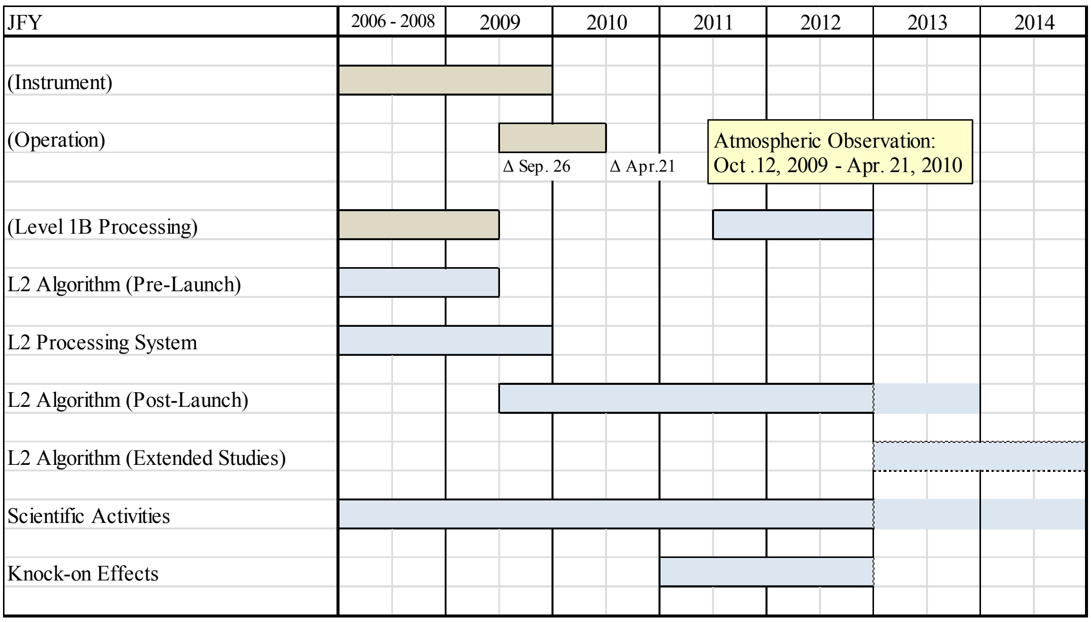
Schedule, resources and implementation

28 March 2013

Takuki SANO, sub-manager of SMILES-ISAS team
ISS Science Project Office,
Japan Aerospace Exploration Agency

1

Schedule of SMILES Project



2

Development of SMILES Data Processing System (DPS)

- Development of early version was completed in the spring of 2009 (before SMILES launch).
- Processing speed: comparable with real-time observation (ex. 1 min for 1 scan (53 sec.)).
- Early version of retrieval algorithm results in “qualitatively-correct” profiles.

(Self-rating)

- DPS team, computer resources, budget, ... were sufficient.

3

Operation of SMILES DPS

- L1B Operation:
  - Not designed for reprocessing (only for real-time processing)
  - Offline L0 data transfer (in the same operation room, with disc media)
  - Processing speed: 1 mo. for 6 mo. data
- L2 Operation:
  - 3-4 versions of reprocessing including validation
  - Processing speed: 1.5 mo. for 6 mo. data
  - Lack of schedule management

(Self-rating)

- Whole operation was almost acceptable.
- Machine resources should be enhanced, esp. for L1B processing.

4

Improvement of SMILES DPS

- DPS-L1 were based on the validation of L2 data retrieved from the new L1B sample data.
  →Reliable improvement, but some waste of time for discussion between L1 and L2 team.
- DPS-L2 initially had several problem:
  - Target data of validation; satellite, ground-based observation, or model calculation ?
  - Difficulty of discrimination of L1B- and L2-origin problem in L2 retrieval error

(Self-rating)

- Improvement of DPS-L1 and L2 are acceptable, from the point of view of 3-year reprocessing work.
- DPS-L2 team would demand more 2-year extension of re-reprocessing study to fulfill SMILES' potential.

5

Data Distribution

- Service of preliminary data (v1.0 – v1.3, v2.0) to RA researchers (2010/1 -)
- Public release (v2.1) via SMILES project website (2012/3 -)
- Public release (after v2.4) via ISAS data center (2013/10 -)

(Self-rating)

- It is necessary to establish long-term data distribution scheme (system) in ISAS/JAXA.

6

Science Team / Workshops / Outreach

- JAXA manages science team activity in order to encourage RA (Research Announcement) –based research themes with SMILES data.
- SMILES workshops were held in 2008, 2010 and 2011.
- Operation of SMILES website is ongoing.
  - http://smiles.tksc.jaxa.jp/
  - http://darts.isas.jaxa.jp/iss/smiles/ (for long-term data archiving)

(Self-rating)

- Efforts for these management works with minimum staffs and limited budget can be recognized.

7

SMILES workshop 2010

- On 1-2 March 2010, held at ISAS/JAXA (Sagamihara, Japan)
- About 50 participants (10 of them are from oversea)

8

Outreach (cont.) - Publications

(2013) 8 articles *(4: accepted, 4: in the pipeline)*
other 2 articles in preparation

(2012) 8 articles

(2011) 2 articles

(2010) 5 articles

(2008) 1 article

(- 2006) 14 articles

Total 34 peer-reviewed papers since 2000.
(Instrument: 16, Retrieval & Spectroscopy: 14, Science: 4)

9

Outreach (cont.) – Ph.D. Thesis

- Takatoshi Sakazaki (2013), "Studies on diurnal variations in dynamical fields and ozone field in the stratosphere", Hokkaido Univ.
- Ochiai, Satoshi (2013), "Calibration and Evaluation of Submillimeter-Wave Radiometers for Atmospheric Observation", Osaka Prefecture Univ.
- Kuwahara, Toshihisa (2012), "Study of stratospheric chlorine monoxide and water vapor based on ground-based millimeter-wave observations over Atacama highland, Chile.", Nagoya Univ.
- Takahashi, Chikako (2012), "Development of the retrieval algorithm and capability study of high-precision ozone measurement for JEM/SMILES", Nagoya Univ.
- Verdes, Carmen (2002), "Deriving Atmospheric Temperature and Instrumental Pointing From Millimeter/Sub-Millimeter Limb Sounding Measurements.", Univ. of Bremen.
- Bühler, Stefan (1998), "Microwave Limb Sounding of the Stratosphere and Upper Troposphere.", Univ. of Bremen.

10

Total self-rating of SMILES project in ISAS/JAXA

- Implementation of scientific activities with minimum human resources and limited budgets can be acknowledged.
- JAXA/ISAS should maintain SMILES' scientific activities (writing papers, entry to international conferences, and holding SMILES workshops); which will continue for 2 years (at first).
- DPS-L2 team will apply for competitive funds in order to keep our studies; but also we expect ISAS/JAXA will secure some budget (TBD) for re-reprocessing of L1B/L2 data.

11

Achievement of "Success Criteria" (defined inside JAXA)

	Observation	Science
Minimum Success	To obtain valid spectrum data for over 1 day **[Achieved]**	To retrieve vertical distribution of ozone, HCl and ClO with more precision than any existing observations **[Achieved]**
Full Success	To obtain valid spectrum data for 1 year **[Partly achieved]**	To retrieve global distribution and diurnal variation of atmospheric minor constituents including the species which has been rarely observed **[Achieved]**
Extra Success	To obtain valid spectrum data for over 1 year **[Not achieved]**	To detect unexpected distribution of minor constituents and/or atmospheric phenomenon **[Partly achieved]**

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Core Members of SMILES DPS-L2 and Science (As of Mar., 2013)

- Principle Investigator
  - M. Shiotani
- JAXA/ISAS
  - M. Takayanagi (Manager)
  - T. Sano (Sub-manager)
  - M. Suzuki (Science)
  - K. Imai (Validation Analysis; from Tome R&D)
- Fujitsu FIP (Contractor with JAXA)
  - C. Takahashi (Manager)
  - C. Mitsuda (Algorithm Implementation)
  - Y. Inoue (Data Product Operation)
- Kyoto Univ.
  - E. Nishimoto (Database Improvement)
  - Y. Naito (Climatology analysis)
- Chiba Univ.
  - N. Manago (Algorithm Improvement; former JAXA/ISAS staff)
- Cooperative Members
  - H. Ozeki (Spectroscopy)
  - H. Akiyoshi, D. Kinnison (Model calculation)
  - N. Nishi, M. Fujiwara, T. Sakazaki (Meteorology)
  - K. Takahashi, T. Imamura (Chemistry)

13

RA Research Theme List (1/5)

Principal Investigator (Research Organization)	Research theme	
Yvan Orsolini (NILU, Norway)	Analyses and model comparison of JEM/SMILES observations of key minor constituents involved in stratospheric ozone chemistry	
William Read (JPL, USA)	JEM/SMILES Cloud/Humidity Products	
Arno de Lange (SRON, Netherlands)	JEM/SMILES validation by the balloon instruments TELIS and MIPAS-B	
Ian Boyd (NIWA, NZ)	Validation of JEM/SMILES Ozone Measurements by Ground Based Microwave Ozone Radiometers and Other Instruments at Two NDACC Sites	
Robert A. Stachnik (JPL, USA)	JEM/SMILES Validation using atmospheric observations by the JPL balloon-borne remote sensor suite	
Masatomo Fujiwara (Hokkaido Univ.)	Validation of ozone measured with the Superconducting Submillimeter-Wave Limb-Emission Sounder(SMILES) by ozonesonde measurements	

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RA Research Theme List (2/5)

Principal Investigator (Research Organization)	Research theme	
Joachim Urban (Chalmers Univ., Sweden)	Collaborative research based on atmospheric observations from SMILES and Odin	
Kaley Walker (Univ. of Toronto, Canada)	Validation of JEM-SMILES Measurements Using Infrared Fourier Transform Spectrometer Data Sets	
Yasuko Kasai (NICT)	JEM/SMILES L2 Research Processing, Validation and Science	
Masato Shiotani (Kyoto Univ. RISH)	Comparing the SMILES data with those from the Microwave Limb Sounder aboard the EOS Aura	
Tomoo Nagahama (Nagoya Univ. STE)	Monitoring of Mesospheric Composition Change associated with Solar-Terrestrial Environment Changes	
Toshihisa Kuwahara (Nagoya Univ. STE)	Investigation of diurnal and seasonal variations of stratospheric ClO based on ground-based millimeter-wave observations validated by the comparison with JEM/SMILES data	

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RA Research Theme List (3/5)

Principal Investigator (Research Organization)	Research theme	
Koji Imai (TOME R&D Inc./JAXA)	Stratospheric methyl cyanide (CH3CN) from JEM/SMILES	
Makoto Suzuki (JAXA-ISAS)	Method of diurnal analysis for sun-nonsynchronous observation system using SMILES data	
Jana Mendrok (NICT)	Tropospheric ice cloud measurements from SMILES - Retrieval, validation, and science	
Satoshi Ochiai (NICT)	SMILES Level 1 Calibration (SMILES Level 1 Calibration)	
Satoshi Ochiai (NICT)	Ozone and ClO validation by millimeter-wave radiometer at Alaska	
Takafumi Sugita (NIES)	Quantitative evaluations of inorganic chlorine chemistry in the stratosphere using a photochemical model	
Kiyotaka shibata (MRI)	Study of zonally asymmetric distribution of ozone and related chemical species: Comparison between the SMILES data and the MRI chemistry-climate model data	

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RA Research Theme List (4/5)

Principal Investigator (Research Organization)	Research theme	Late Proposal
Hideaki Nagajima (NIES)	Validation of JEM/SMILES O3, O3-isotope, HCl, and HNO3 profiles with ground-based FTIR spectrometers in Rikubetsu and Tsukuba	
Makoto suzuki (JAXA-ISAS)	Stratospheric SO2 observation from JEM/SMILES	
Mitsuteru Sato (Hokkaido Univ.)	Detection of the chemical effects caused by solar and TLE activities at the middle atmosphere from the SMILES observation	
Lawrence E. Flynn (NOAA/NESDIS)	Comparisons of ozone profiles and assimilation products from SMILES with those from SBUV/2	x
Francois Hendrick (Belgian Institute for Space Aeronomy)	Validation of JEM/SMILES BrO, HCl, and HNO3 measurements using ground-based instrument observations	x
Alexei Rozanov (Univ. of Bremen)	Cross- validation and quality improvement of vertical distributions of O3 and BrO number density retrieved from SMILES and SCIAMACHY measurements	x

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RA Research Theme List (5/5)

Principal Investigator (Research Organization)	Research theme	Late Proposal
Ding-Yi Wang (Univ. of New Brunswick)	Study of Stratospheric Dynamical Processes and Ozone Variations by Space-Based Multi-Sensor Datasets	x
Naoko Saitoh (Center for Environmental Remote Sensing, Chiba University)	Combined use of JEM/SMILES and GOSAT products for cross-validation of stratospheric minor species and study on stratospheric ozone chemistry in the Arctic	x
Shingo Watanabe (Research Institute for Global Change/JAMSTEC)	Cross-validations of SMILES level 2 products against results of chemistry climate models	x

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5. L2 Data Processing and Product Status

Makoto Suzuki*2
Chihiro Mitsuda*1, Takuki Sano*2, Naohiro Manago*3,
Eriko Nishimoto*2,4, Yoko Naito*4, Chikako Takahashi*1,
Koji Imai*5, Masato Shiotani*4

*1: Fujitsu FIP , *2: ISAS/JAXA, *3: Chiba Univ., *4: Kyoto Univ., *5: TOME R&D

1

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

5

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

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Mission Plan: Antenna Pattern

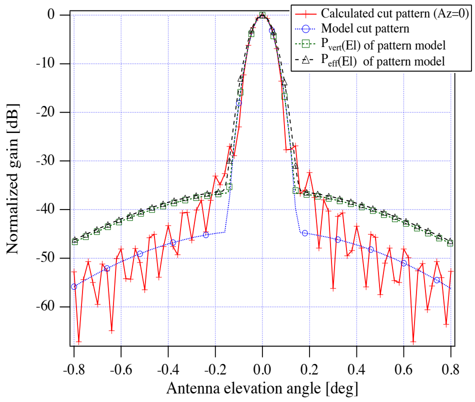
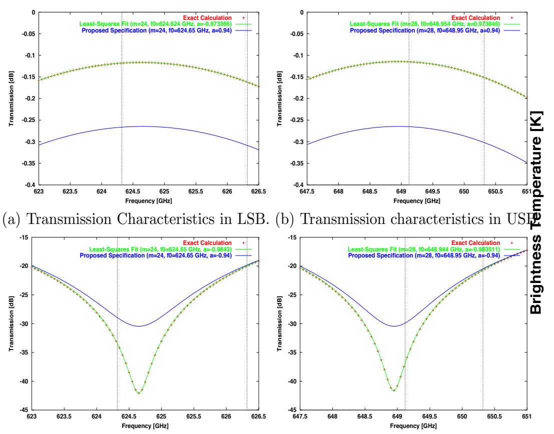


Figure 3.18 Effective antenna response pattern.

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



(a) Transmission Characteristics in LSB. (b) Transmission characteristics in USB.

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

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.

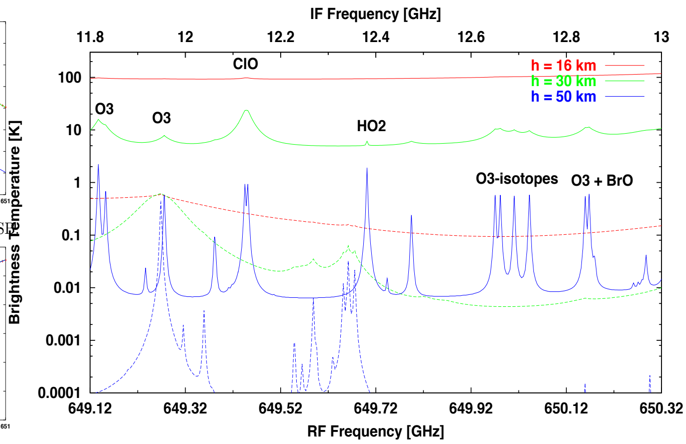


Figure 3.31 The effect of the image contributions in Band-C.

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

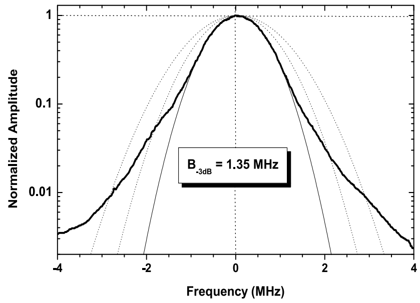


Figure 3.33 Frequency response function of the SMILES/AOS. The typical resolution bandwidth is 1.35 MHz.

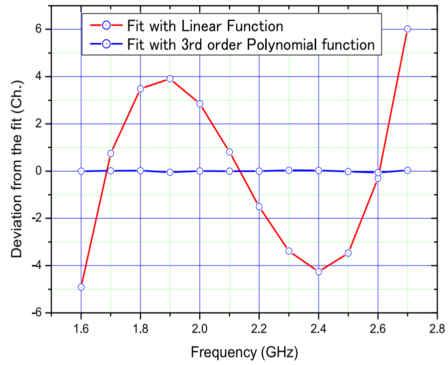


Figure 3.34 Residuals from the frequency fit with comb generator. 1 Ch. corresponds to approximately 0.8 MHz.

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.

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

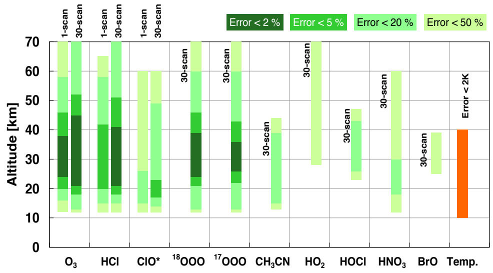

Figure 1.4 Altitude coverage of the JEM/SMILES data estimated from preliminary results of simulation studies assuming 0°N standard profile for each molecular species except for ClO for which the standard profile for polar region is assumed. Refer to Chapter 4 for more details.

SMILES Mission Plan v2.11 (2002)

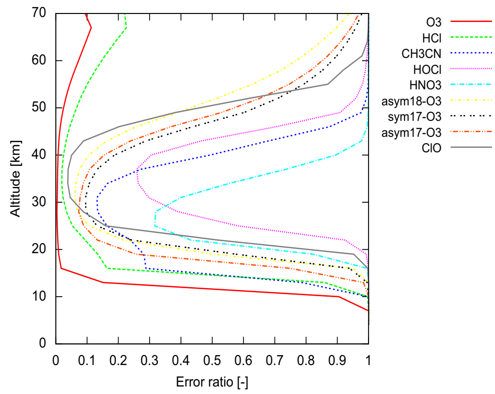

Fig. 9. Retrieval precision of target species that can be retrieved from single-scan data.

Takahashi, Ochiai, Suzuki (2010)

A priori accuracy
10° latitude bin, monthly a priori

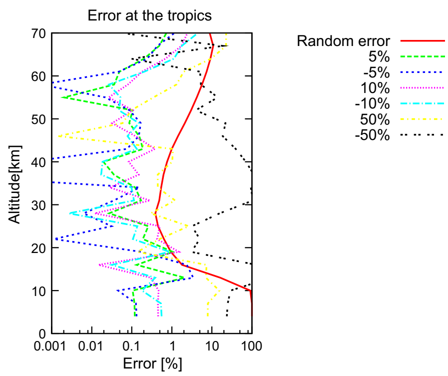

Fig. 5. Estimations for the influence of priori profiles in O_3 retrieval (in this case, a priori profiles are same as initial profiles). The solid red line is the random error of O_3. The other lines are additional errors between the true profiles of O_3 and the retrieved profiles of O_3 that are the final results of the iteration process in the cases where the differences between the a priori profiles and true profiles are ±5%, ±10%, and ±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.

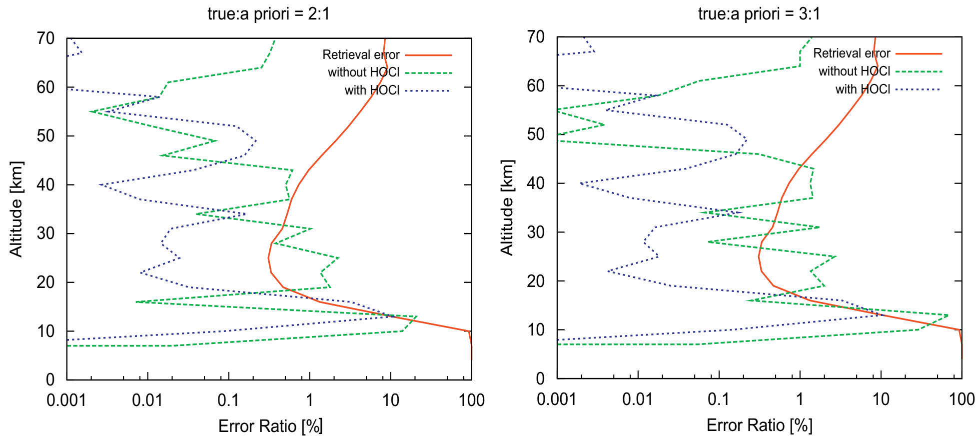

Fig. 2. Simultaneous retrieval of ozone and HOCl. The red (solid) line indicates the retrieval precision in ozone retrieval, the green (dashed) line indicates the incremental error in ozone retrieval without HOCl, and the blue (dotted) line indicates the incremental error in ozone retrieval with HOCl.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

Takahashi, Ochiai, Suzuki (2010)

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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.

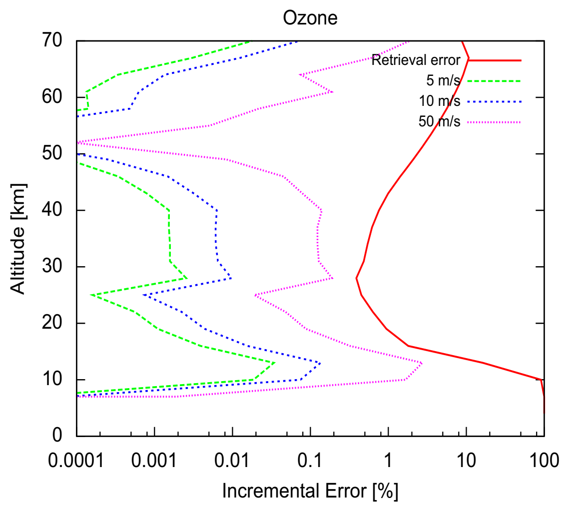

Fig. 3. Effect of wind. The red (solid) line indicates the retrieval precision of ozone. The other lines indicate the error due to the difference between the reference profile and the true profile of wind. (The wind velocities for the pink (fine dotted), blue (dotted), and green (dashed) profiles are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

Takahashi, Ochiai, Suzuki (2010)

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

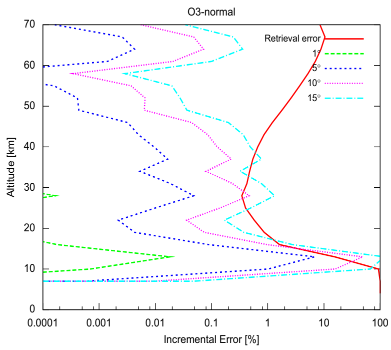

Fig. 4. Error due to inclination of antenna scan axis. The red line (solid) indicates the retrieval precision of ozone. The other lines indicate the error due to the inclination of the antenna scan axis. The inclinations of the antenna scan axis in the aqua blue dashed-dotted, pink (dotted), dark blue, and green (dashed) profiles are 15°, 10°, 5°, and 1°, respectively. The definition of the incremental error is the same as that in Fig. 2. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Takahashi, Ochiai, Suzuki (2010)

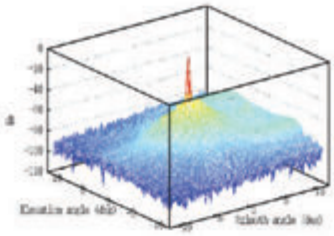

Fig. 3 Two dimensional (Elevation, Azimuth) SMILES antenna pattern.

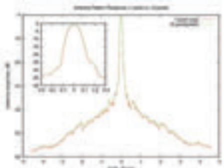

Fig. 4 One dimensional antenna pattern in elevation axis without antenna motion (dark), and with antenna motion (light).

Suzuki et al., (2011)

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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.

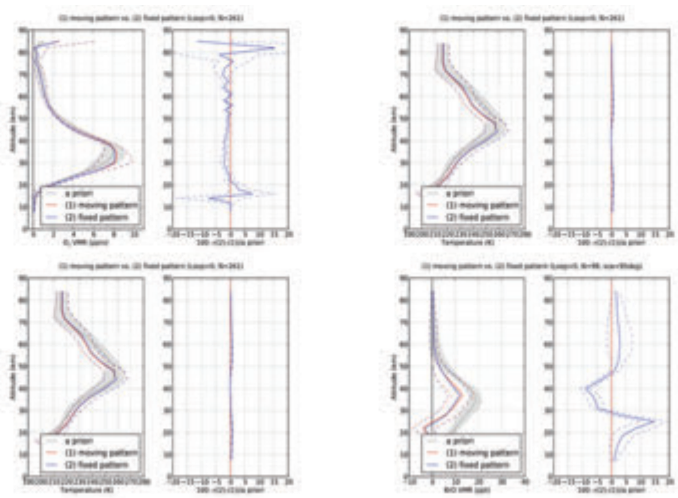

Fig. 5 Averaged retrieved profiles (red: moving antenna, blue: fixed antenna), relative difference normalized to a priori of L2 ver. 1.3 O_3 (upper left), temperature (upper right), HCl (lower left) and BrO from SMILES Band A (lower right). 261 observations are averaged in Oct. 12, 2009 at equatorial region N10-S10.

Suzuki et al., (2011)

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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.

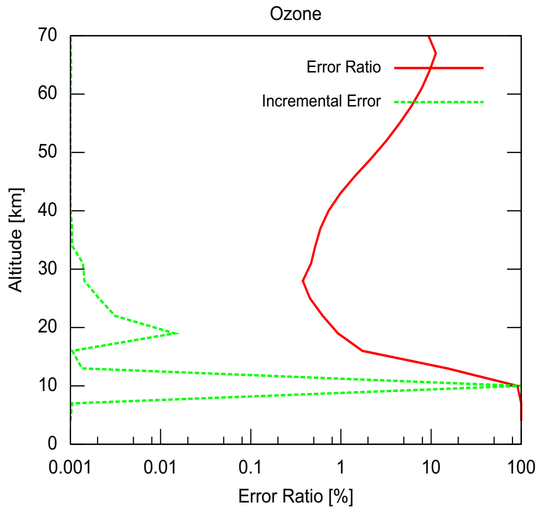

Fig. 5. Error due to line selection. The red (solid) line is the retrieval precision of ozone, and the green (dashed) line indicates the incremental error in retrieved ozone due to line selection. The definition of the incremental error is the same as that in Fig. 2.

Takahashi, Ochiai, Suzuki (2010)

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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.

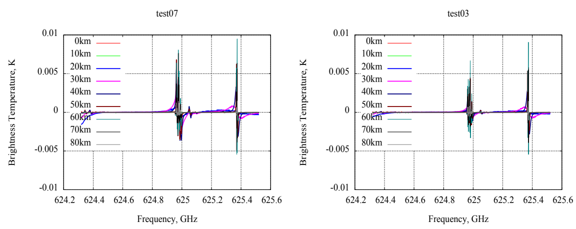
Grid pitch of integration of AOS response function

(AOS1)

Freq. difference from center	Ratio of sensitivity	Freq. step
-8.0 ～ -2.8	< 0.02	0.4 MHz
-2.8 ～ 2.4		0.2 MHz
2.4 ～ 8.0	< 0.01	0.4 MHz

(AOS2)

Freq. difference from center	Ratio of sensitivity	Freq. step
-8.0 ～ -2.8	< 0.02	0.4 MHz
-2.8 ～ 2.4		0.2 MHz
2.4 ～ 6.0	< 0.01	0.4 MHz



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

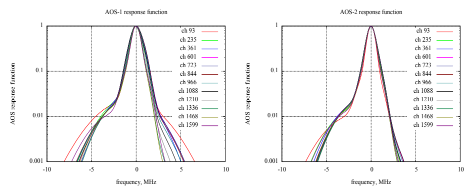


図 3.9 AOS 応答関数（左：AOS1, 右:AOS2）。横軸はチャンネル中心からの周波数の差。各線はチャンネルが異なる。

FY2009 FIP progress report to JAXA (Mar. 2009)

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~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)

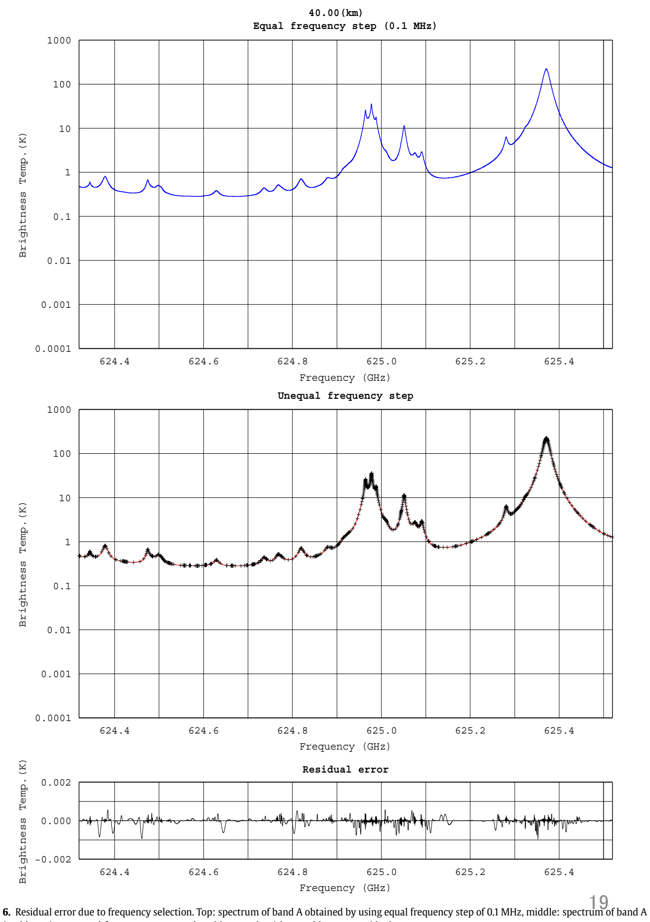


Fig. 6. Residual error due to frequency selection. Top: spectrum of band A obtained by using equal frequency step of 0.1 MHz, middle: spectrum of band A obtained by using unequal frequency steps produced by our algorithm, and bottom: residual error.

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

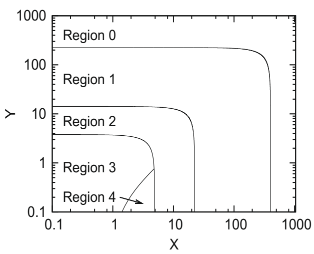


Fig. 2. The five regions in the x–y plane (region 0: Lorentz approximation; region 1: Gauss–Hermite quadrature 2 points; region 2: 4 points; region 3: 5 points; and region 4: 7 points, respectively). The regions 1–4 are originally relevant for Humlicek's approximation of the Voigt profile function.

Table 1
Maximum and standard deviation of relative error between Armstrong's and other algorithms for the narrow and the wide range.

Algorithm	Narrow range		Wide range	
	ϵ_{max}	ϵ_{std}	ϵ_{max}	ϵ_{std}
This work	9.38×10^{-5}	1.31×10^{-5}	2.52×10^{-5}	7.88×10^{-7}
Humlicek	4.88×10^{-3}	1.20×10^{-3}	8.41×10^{-5}	3.09×10^{-6}
Hui	1.05×10^{-3}	1.15×10^{-4}	1.03×10^{-5}	1.80×10^{-7}

Table 2
Computing time in seconds for the narrow and the wide range.

Algorithm	Narrow range $\times 10^2$ (s)	Wide range $\times 10^3$ (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.

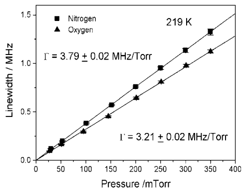


Fig. 2. Pressure dependence of line broadening of the 625.371 GHz line of O_3. Error bars indicate 1σ limits.

O3, pressure broadening.
Yamada and Amano (2005)

Table 1
Halfwidth parameters of BrO

Line/gas	624.77 GHz		650.17 GHz	
	γ_0 (MHz/Torr)	n	γ_0 (MHz/Torr)	n
N_2	3.24 (5)	−0.76 (5)	3.20 (7)	−0.84 (7)
O_2	2.33 (6)	−0.93 (7)	2.41 (6)	−0.70 (7)

γ_0 is the pressure broadening coefficient at 296 K, and n is the temperature dependence exponent.

Pressure broadening of BrO
Yamada et al. (2003)

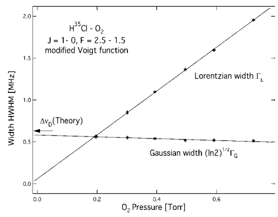


Fig. 2. The Lorentzian widths Γ_L and the Gaussian widths Γ_G of the $H^{35}Cl$ $J = 1$–0, $F = 2.5$–1.5 transition for the oxygen-gas effect, obtained by *modified* Voigt profile analysis, are plotted versus O_2 pressure. To compare with the theoretical Doppler HWHM, the Gaussian widths are presented here as the HWHM, i.e., $(\ln 2)^{1/2}\ \Gamma_G$. The Γ_G value decreases with the increase of pressure, and are smaller than theoretical value calculated for the temperature. The error bars for the width indicated are one standard deviation estimated by the profile fit procedure. The horizontal error bars indicate the pressure changes during the measurement.

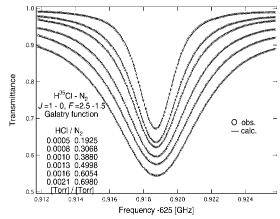


Fig. 3. Typical line profiles measured for the $H^{35}Cl$ $J = 1$–0, $F = 2.5$–1.5 transition in the N_2-broadening experiments is reproduced. Displayed are transmittance spectra, which are the transmission intensity divided by the background (incident) radiation. The open circles represent observed values and the solid lines are the best-fit Galatry profiles determined by the LS analysis.

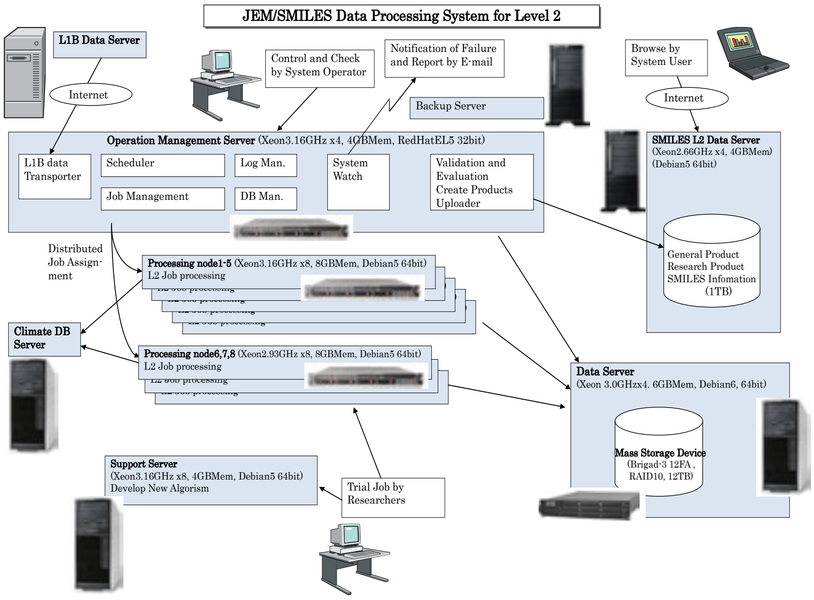
Table 1

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

L2 Prelaunch Algorithm satisfied Mission Plan requirements. Even though calculating 10^4 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



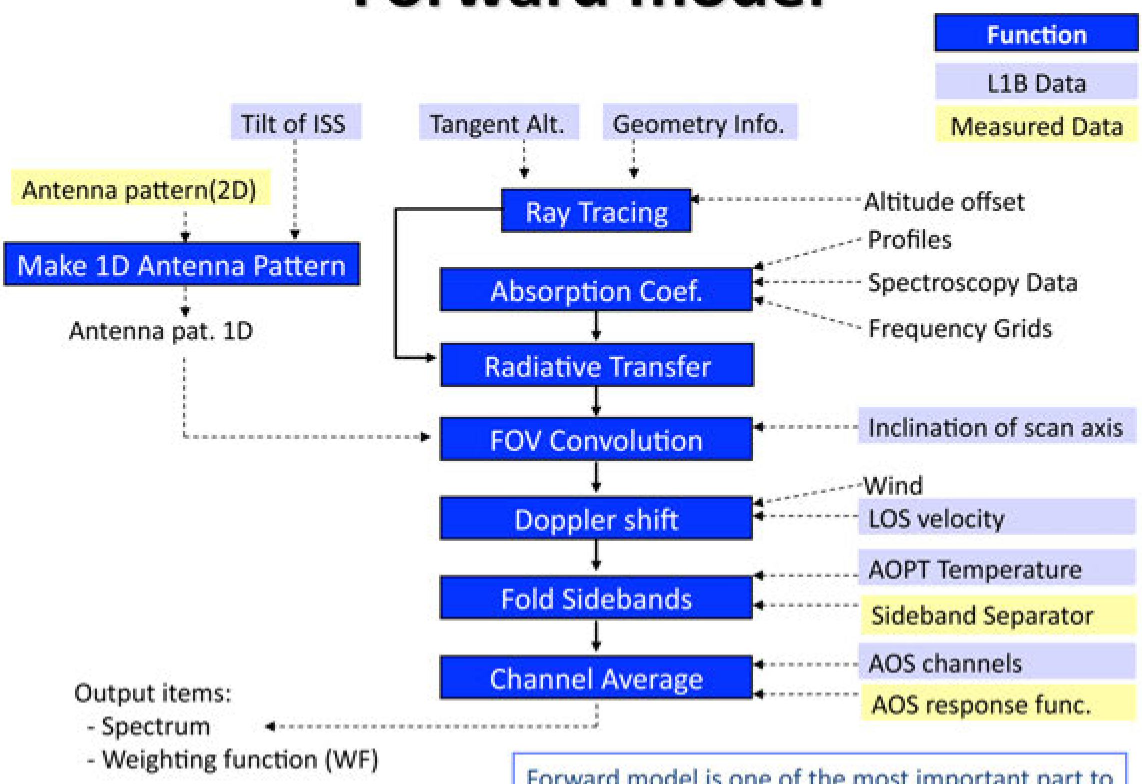
L2 System CPU Configureation

	Operation 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
Type	HP Proliant DL360G5	HP Proliant DL360G5	HP Proliant DL160G6	HP Proliant ML350G5	HP Proliant ML350G5	HP xw8600 CT	Plat'Home TrusRAID	Brigad-3 12FA	HP dc7900	HP ProCurve	APC SmartUPS1500
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)

Forward model



Forward model is one of the most important part to determine the accuracy and its computing cost

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Inversion model

- **Optimal Estimation Method + Tikhonov Regularization Method**
  - **Observation vector** $\mathbf{y} = \mathbf{f}(\mathbf{x}) + \varepsilon$

    (x : true、 ε : observation noise 、 f : Forward Model)
  - **Deriving the results which minimize** χ^2

$$\chi^2 = [\mathbf{y}-\mathbf{f}(\mathbf{x})]^T \mathbf{S}_\varepsilon [\mathbf{y}-\mathbf{f}(\mathbf{x})] + [\mathbf{x}-\mathbf{x}_a]^T \mathbf{S}_a [\mathbf{x}-\mathbf{x}_a] + \alpha[\mathbf{x}-\mathbf{x}_a]^T \mathbf{L}^T\mathbf{L}[\mathbf{x}-\mathbf{x}_a]$$

(x_a : a priori, S_a : covariance of a priori, S_y covariance of observation noise,

α: regulization factor, L: Regulization matrix)

- **Non-linear case (Levenberg-Marquardt Method)**

$$\mathbf{x}_{i+1} = \mathbf{x}_i + \left\{\mathbf{S}_a^{-1} + (\alpha\mathbf{L}^T\mathbf{L})^{-1} + \mathbf{K}_i^T\mathbf{S}_y^{-1}\mathbf{K}_i + \gamma\mathbf{S}_a^{-1}\right\}^{-1} \left\{\mathbf{K}_i^T\mathbf{S}_y^{-1}[\mathbf{y}-\mathbf{f}(\mathbf{x})] + \mathbf{S}_a^{-1}[\mathbf{x}-\mathbf{x}_a] + (\alpha\mathbf{L}^T\mathbf{L})^{-1}[\mathbf{x}-\mathbf{x}_a]\right\}$$

(K_i : Weighting function, γ : Levenberg-Marquardt parameter)

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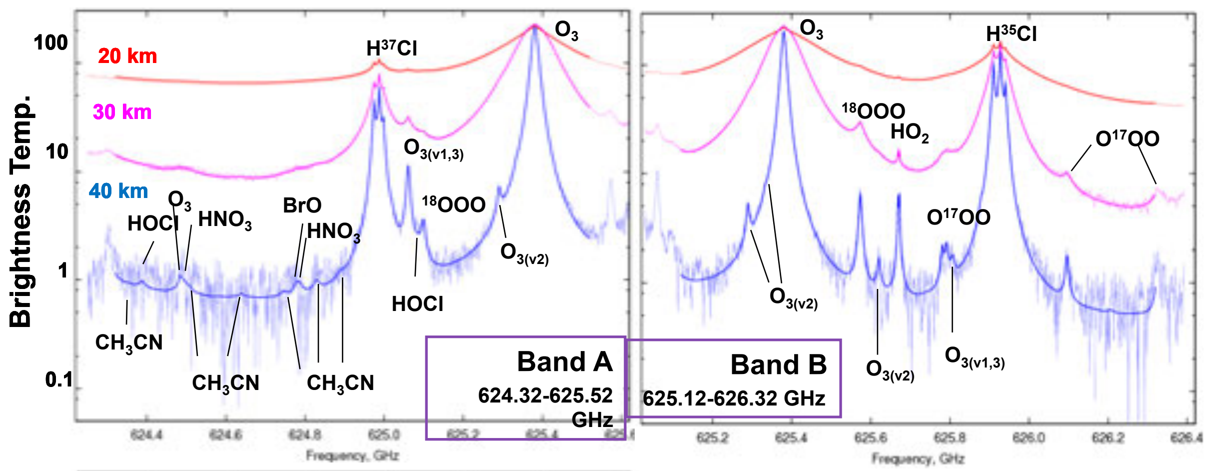
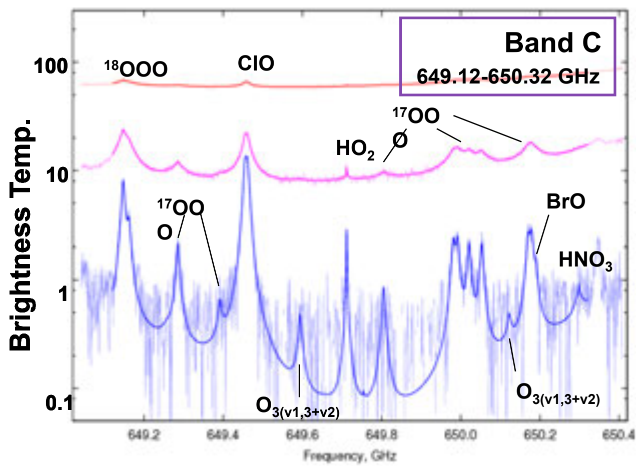
A priori dataset

○: exist, ●: v1.0, ●: v2.4

	Climatology				Nearest grid		
	Aura/ MLS[1]	UARS/ MLS[2]	CCSR/NIES CCM[3]	WACCM4 CCM[4]	GEOS-5[5]	WACCM4 CTM[6]	Aura/ MLS[7]
O_3	●(v1.0) ●(v2.4)		○	○	○	○	○
HCl	●(v1.0) ●(v2.4)		○	○		○	
ClO	●(v1.0) ●(v2.4)		○	○		○	
HNO_3	●(v1.0) ●(v2.4)		○	○		○	
CH_3CN		●(v1.0) ○		○		●(v2.4)	
HOCl	●(v1.0) ○		●(v2.4)	○		○	
HO_2	○		●(v1.0) ●(v2.4)	○		○	
BrO	○		●(v1.0) ●(v2.4)	○		○	
Temp.	○		○	○	●(v1.0) ●(v2.4)	○	●(v2.4)
Pres.	○		○	○	●(v1.0) ●(v2.4)	○	○
Wind			○	○	●(v1.0) ●(v2.4)	○	
H_2O	○		○	○	●(v1.0) ●(v2.4)	○	

*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





Sample spectra

Band A:

- There are strong O3, HCl lines and HOCl, CH3CN lines.. BrO/HNO3 are worse than other band's profiles.

Band B

- There are same O3 line and other HCl lines. HO2, O3 isotopes are observed.
- O17OO lines are located wing of HCl and outside of useful frequency, it is more difficult than other isotopes..

Band C

- There are strong ClO lines and O3 isotopes, BrO and HNO3, HO2 are observed.

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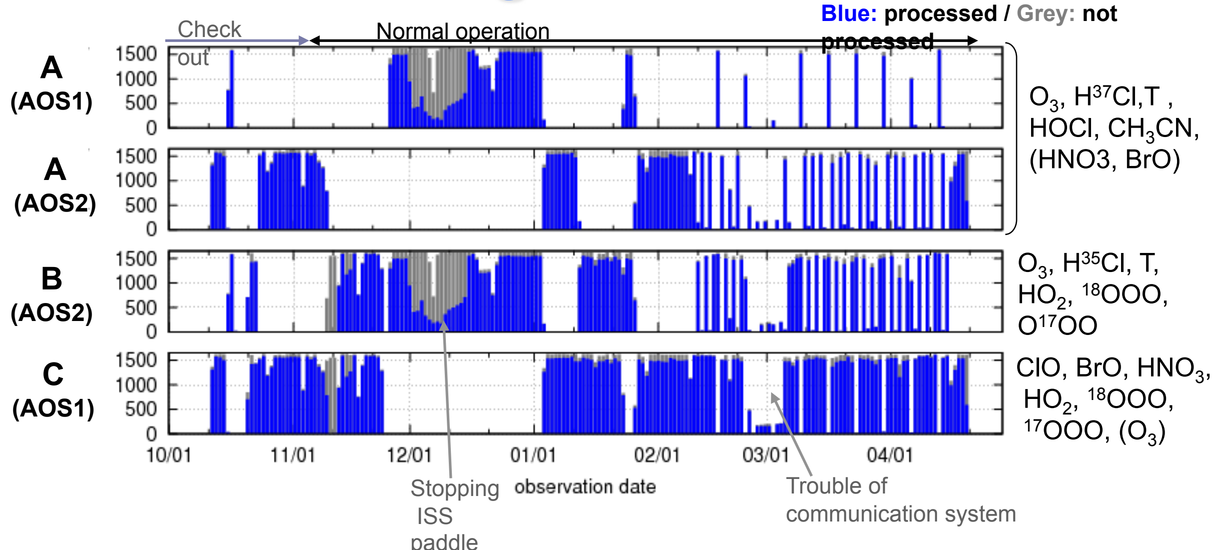
L2 Processing data for each band



- Since SMILES has only 2 receivers, SMILES observed 2 bands simultaneously.
  - 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 SMILES field of view (2009/12/01 – 15), and trouble of communication system of ISS/JEM (2010/02/25 – 03/05).

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v1.0 (005-06-0024) L2 results example. Kikuchi et al. 2010

O_3 and HCl: quite acceptable. Others: need further studies.

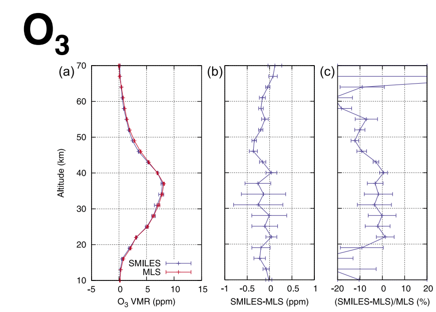

Figure 8. Comparison of coincident SMILES and MLS ozone profiles on 12 October 2009 at northern high latitudes: (a) the mean profiles for SMILES (blue) and MLS (red), (b) the differences between the SMILES and MLS profiles in mixing ratio, and (c) the percentage differences.

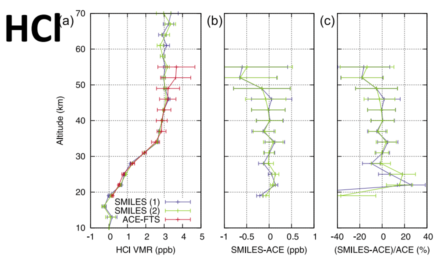

Figure 9. An example of HCl profiles from SMILES and a comparison with that from ACE-FTS: (a) two profiles from SMILES on 12 October 2009, (1) at 5.1°N and 166.5°E (blue), (2) at 7.7°N and 168.4°E (green), and one profile from ACE on 13 October 2009 at 5.2°N and 170.7°E (red) within 24 hr and a distance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

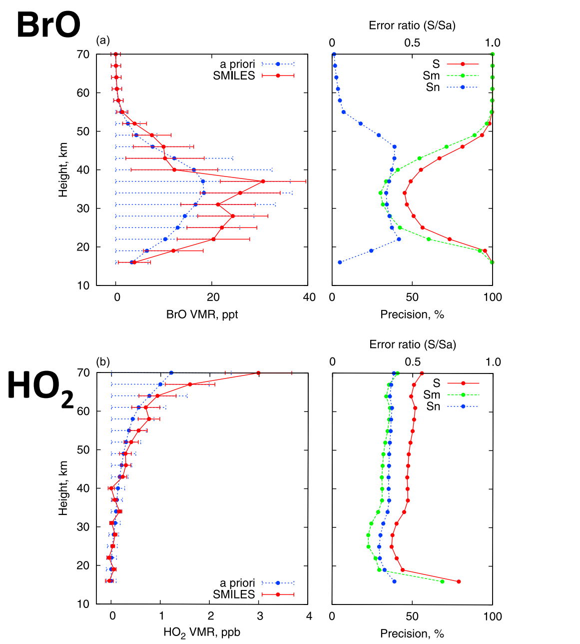

Figure 10. Examples of the retrieved and a priori profiles for (a) BrO and (b) HO_2. Left: Marks and horizontal bars indicate retrieved values and one standard deviation in red, and those for the a priori profile in blue. Right: S, total error; Sm, measurement error; Sn, smoothing error.

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L2 v1.1 validation trial: O_3

Suzuki et al. 2010 (ISPRS Conference Paper)

ACE-FTS **MLS** **MIPAS (IMK)**

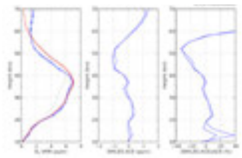

Figure 2. Example of O_3 coincidence; ACE-FTS ver.2.2 (Red) and SMILES (Blue) at latitude 66.0° and longitude 77.5°W on Nov. 13, 2009, profiles (left), absolute difference (middle), and relative difference (right). Two SMILESprofiles are compared with 1 ACE-FTS profile.

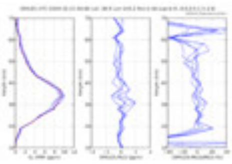

Figure 3. Example of O_3 coincidence; SMILES (red) and AURA/MLS ver.2.2 (Blue) at 30.9°S and 143.2°E on Oct. 23, 2009, similar to Figure 2. One SMILES profile is compared to 5 MLS profiles.

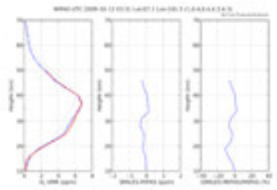

Figure 4. Example of O_3 coincidence; MIPAS-IMK (red) and SMILES (blue) at 67.0°N and 101.5°E on Oct. 12, 2009, similar to Figure 2.

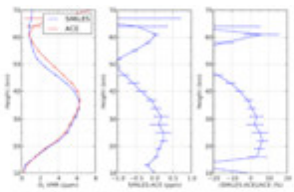

Figure 5. Statistics of 75 O_3 coincidences with 31ACE-FTS (ver.2.2) observations at the 55°N-65°N latitude region.

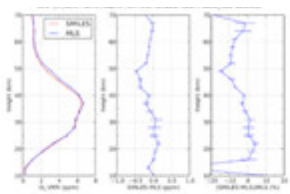

Figure 6. Statistics of 61 O_3 coincidences compared with 284 AURA/MLS (ver.2.2) observations at the 55°N-65°N latitude region.

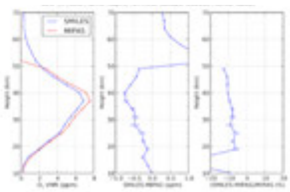

Figure 7. Statistics of 110 O_3 coincidences compared with 52 ENVISAT/MIPAS (MIPAS IML ver.40) observations at the 55°N-65°N latitude region.

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L2 v1.1 validation trial: HCl

Suzuki et al. 2010 (ISPRS Conference Paper)

ACE-FTS **MLS**

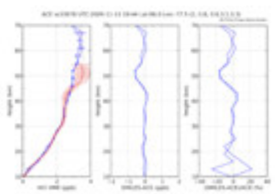

Figure 8. Example of HCl coincidence with ACE-FTS, at the event same as Figure 3.

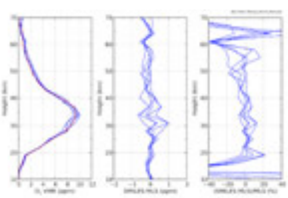

Figure 9. Example of HCl coincidence with AURA/MLS, at the event same as Figure 4.

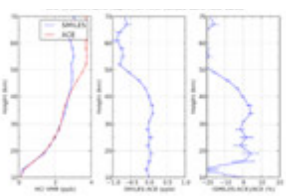

Figure 10. Statistics of HCl coincidence comparison with ACE-FTS at the 55°N-65°N region.

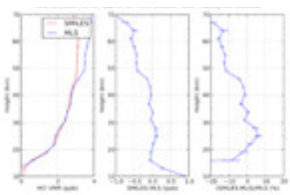

Figure 11. Statistics of HCl coincidence comparison with Aura/MLS at the 55°N-65°N region.

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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

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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.

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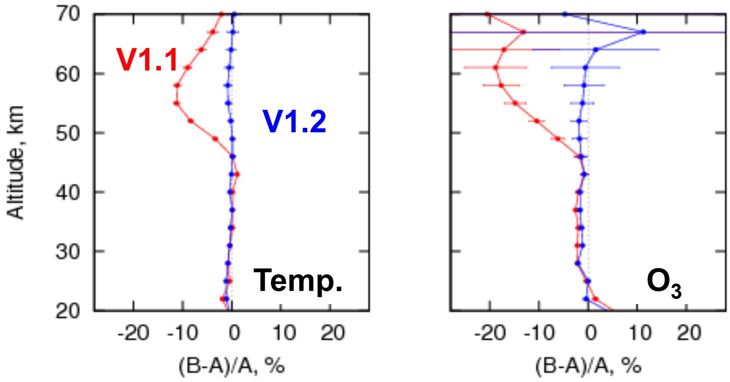
Major improvements in v1.X Series:
Reducing internal inconsistency

Relative Differences of Temperature (left) and O_3 (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.

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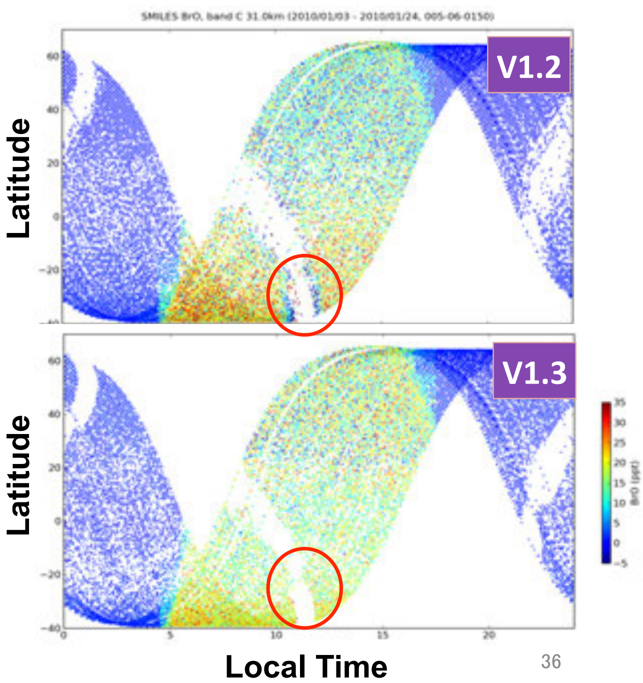
Major improvements (2/2):
flag updates

- 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)



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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.
- **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)

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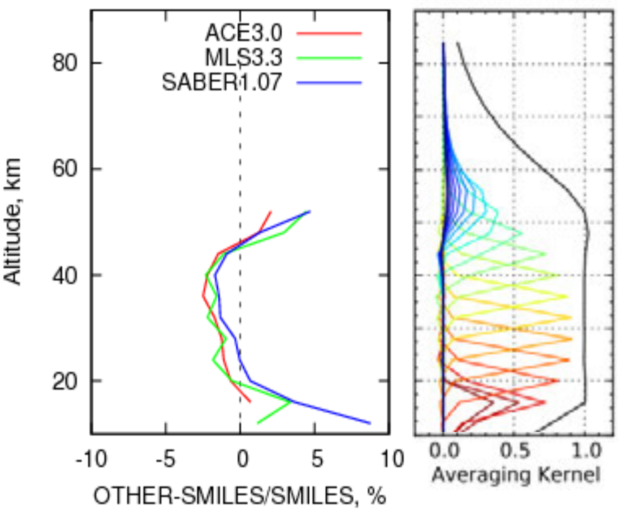
L2 v2.0

Objective:
To reduce temperature bias

– Temperature in v1.3,
  - 55 - km : no information
  - 50-55 km : 5 % lower
  - 20-50 km : 2 % higher than other satellites (ACE, MLS and SABER)
– Since three data are consistent, this difference may be SMILES's bias.
– We recognized that this bias is the largest issue in v1.X series. Temperature is a basic parameter which characterizes the atmospheric structure. Temperature bias influence other products.
– We try 2 approaches to archive this objective.

ACE, MLS, SABER vs. SMILES v1.3

SMILES: band B, N40-N50,
ACE: t < 3h, r < 500km
MLS, SABER: t< 1h, r < 300 km
(Altitude selection: S/Sa < 0.5)



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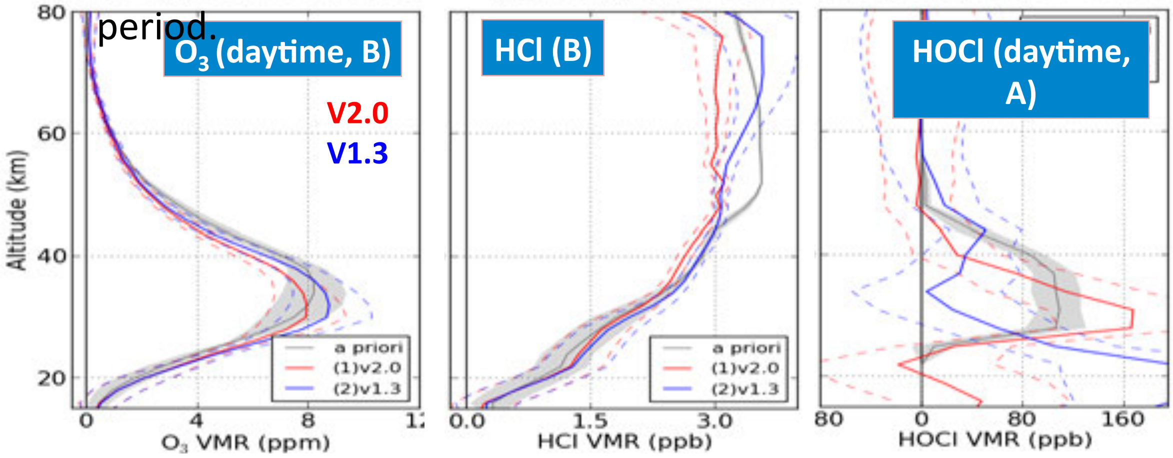
Big impacts of non-linearity correction

Averaged profiles and standard deviation for observation period.



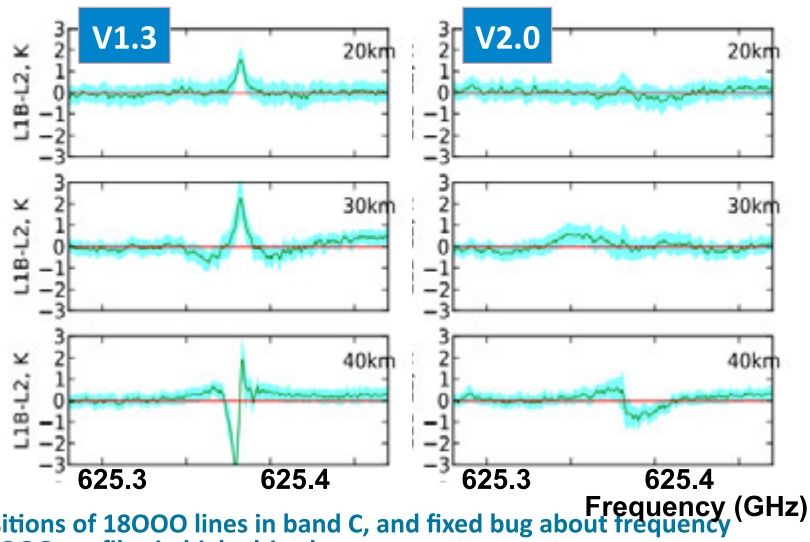
- O_3 and HCl have strong lines in SMILES's bands. These molecules decrease by 5-10 %.
- Since HOCl's lines are located in O3 wing, the profile shape is changed.

Updates of line parameters

- **We start re-check of line parameters.**
- **Preliminary updates were included in v2.0 (O_3 line)**
  - **We changed O3 position and pressure broadening parameter, residuals are reduced.**

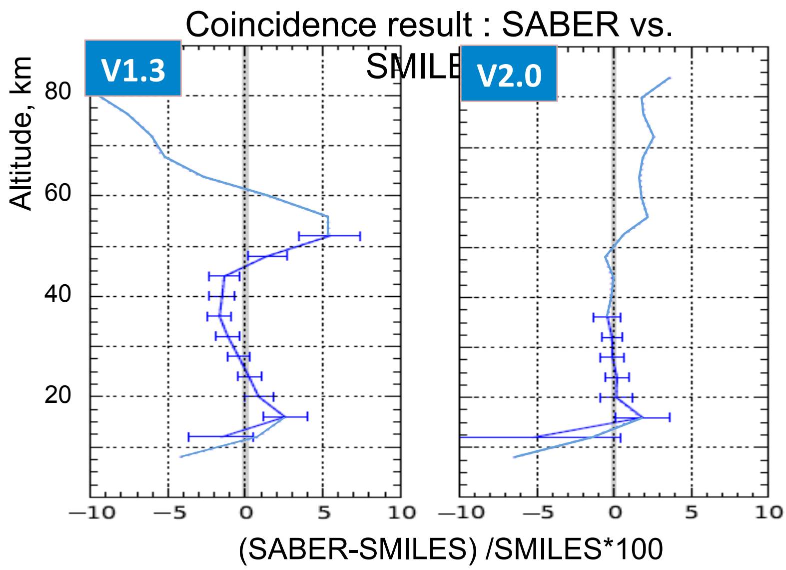
Residual Spectra around O_3 line ,
band A (N=40)
averaged for 1 hour, Asc
(2010/01/04 22:00 – 23:00),

	V1.3	v2.0
Line pos. (MHz)	625371.112 (ref: JPL catalog ver4)	625.371.223 (ref: Ozeki private communication)
γ_{air} (MHz/ hPa), n	2.258 0.77 (ref: MASTER)	2.3078 0.78 (ref: HITRAN2008)



- **We also changed positions of 18OOO lines in band C, and fixed bug about frequency grids. It improved 18OOO profiles in high altitude.**

V2.0: Correcting Temperature profiles



Coincidence condition:
diff t < 1 h
r < 200 km
latitude : S35-S25

Dark blue line:
enough information from observed spectra

Light blue line:
not enough information and return near *a priori* profile

- 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..

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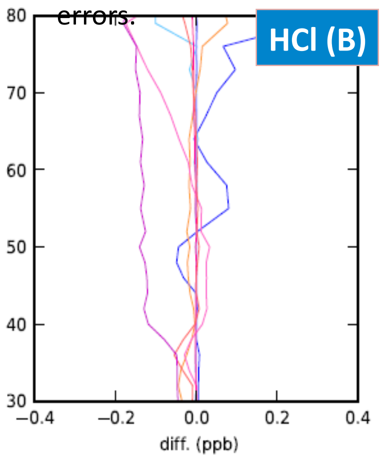
(preliminary) HCl systematic error analysis

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



Retrieval algorithm error
O3 apriori error (20%)
HCl apriori error
H2O apriori error (50%)
Pres. apriori error (5%)
Temp. apriori error (2-5K)
wind apriori error (20m/s)
O3 gamma error (5%)
HCl gamma error (5%)

※ Retrieval algorithm error shows difference between true profiles and unperturbed run. This error associated with retrieval formulation and settings.

- HCl has about 0.2 ppb due to only *a priori* and line parameter's uncertainties.
- In addition, HCl error induced by HCl's γ_{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.

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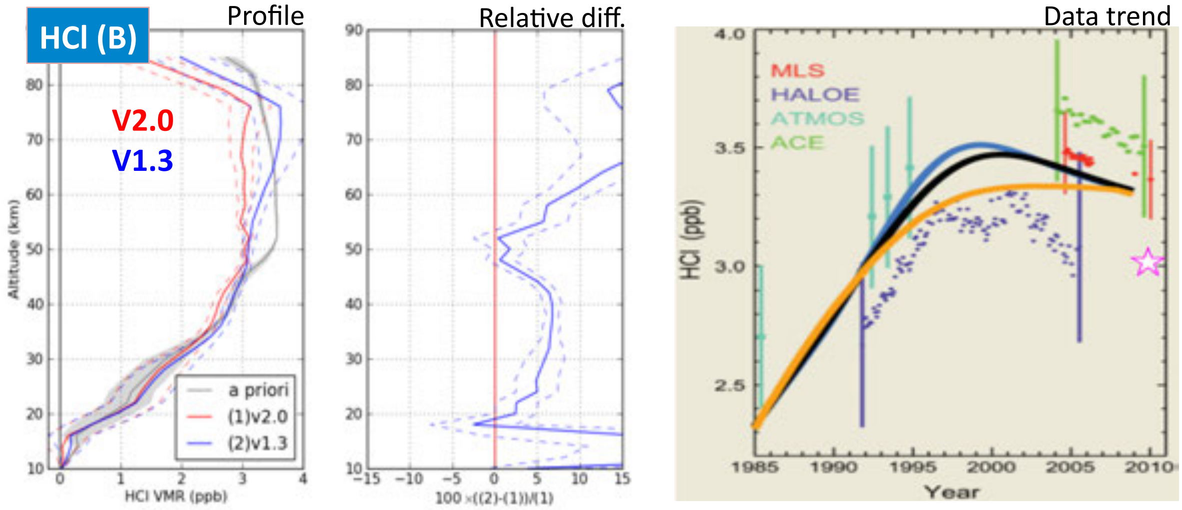
Improvement in HCl products



※These figure show HCl case.
Line formats are same as previous figures.

※This figure shows HCl data trend by WMO report.

- 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))

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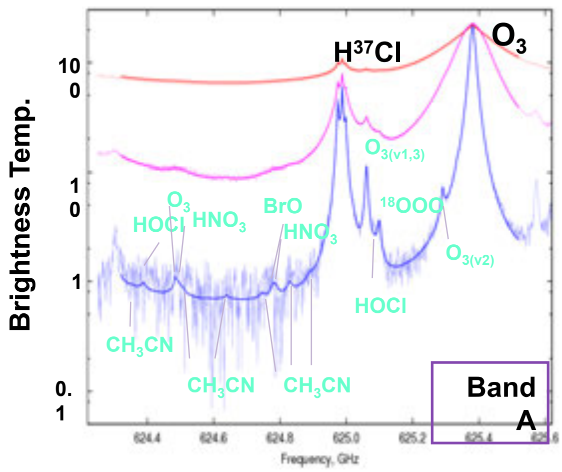
Approach (1/2): for mesosphere

- **Referring more appropriate temperature**
  - SMILES does not measure O_2 emission lines for temperature retrieval, but used other strong lines, O_3 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.

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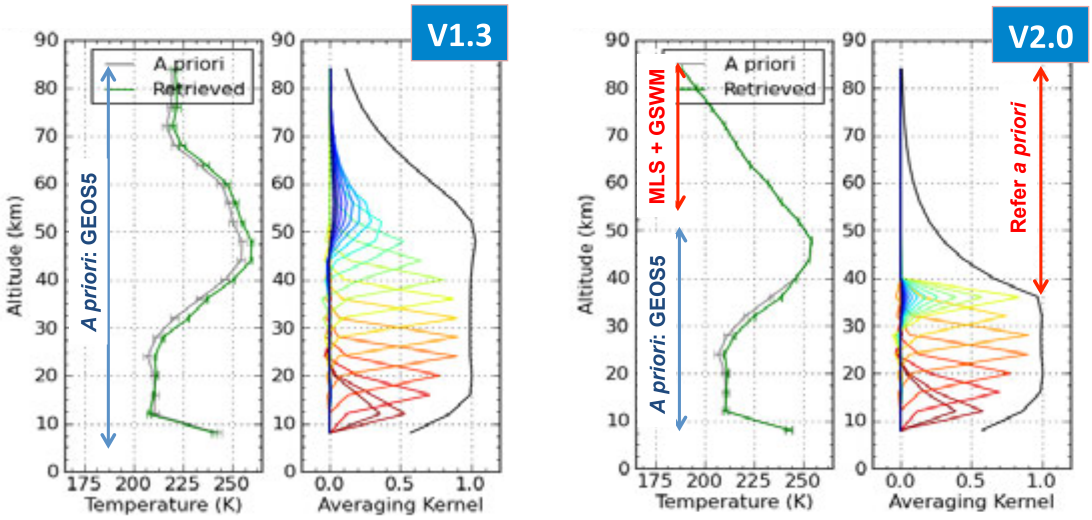
Approach (1/2): for mesosphere (cont.)



In v1.3, GEOS-5 data used as a priori profile in all altitude range.

In v2.0, GEOS-5 data is used as a priori profile in stratosphere and MLS data is used in mesosphere.

- 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.

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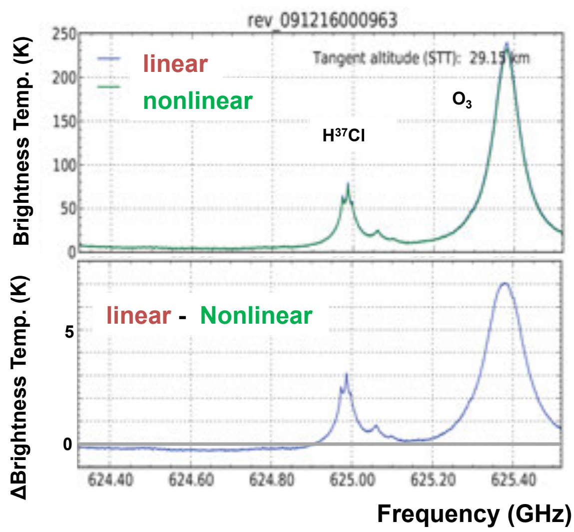
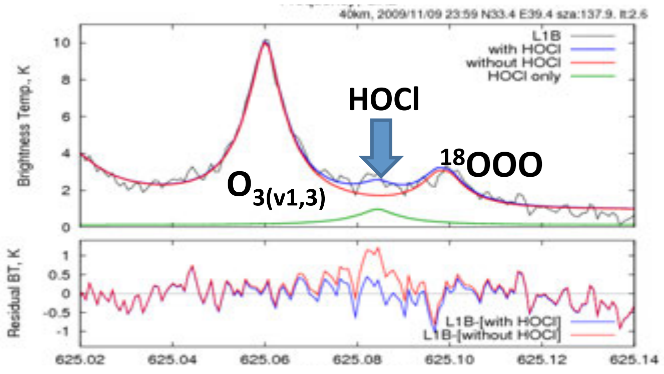
Approach (2/2): for upper stratosphere

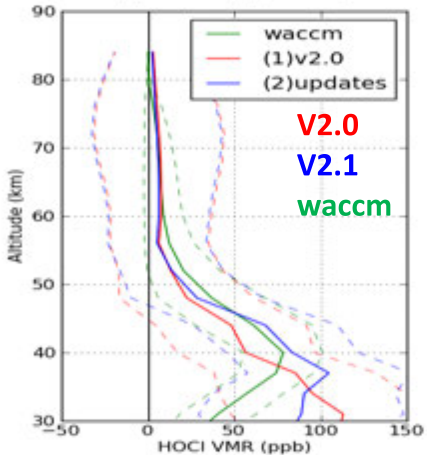
- **Including gain non-linearity in L1B (Ochiai et al., 2011)**

- 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.



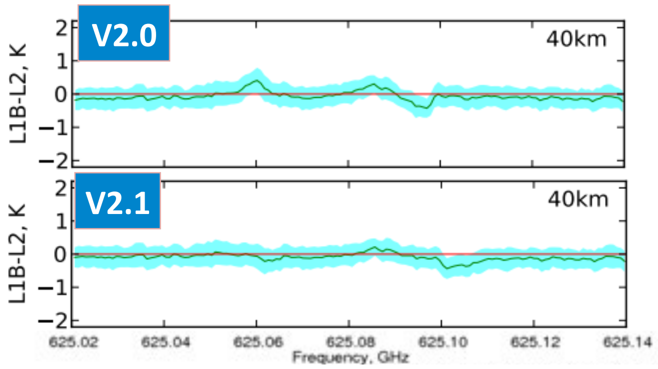
V2.1: Minor update version for HOCl





Residual Spectra around the HOCl line

band A , AOS2 (N=69) averaged for 1day(2010/04/01), Des, lat S45-S35.



- We prepare minor version up for HOCl. Sample spectrum of HOCl is shown in upper figure.
- HOCl is located near $O_{3(v1,3)}$ and ^{18}OOO. In minor update version, parameters of these lines are changed.
  - Residual spectra is compressed.
  - This version will be released in winter.

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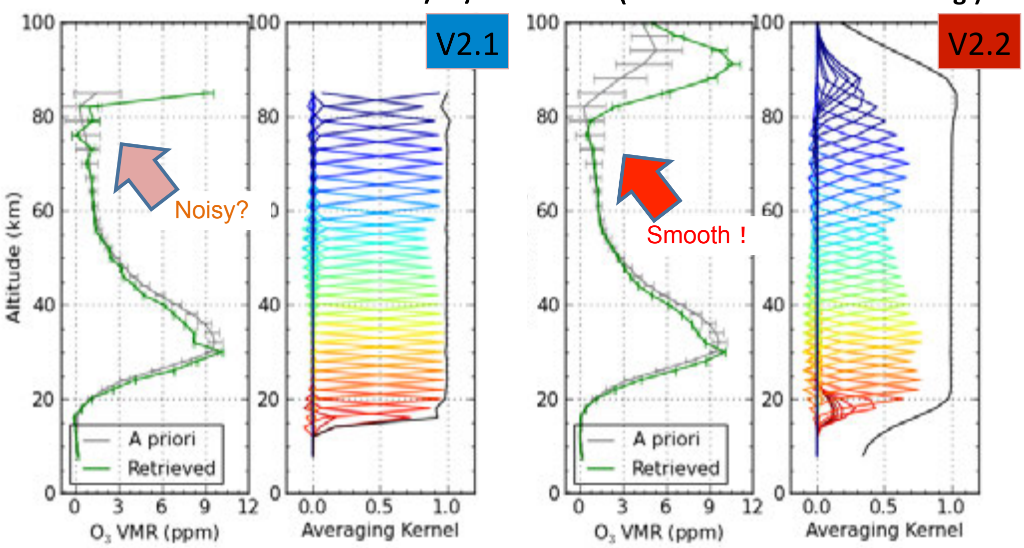
V2.2: improve mesospheric profiles

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.)



- 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.

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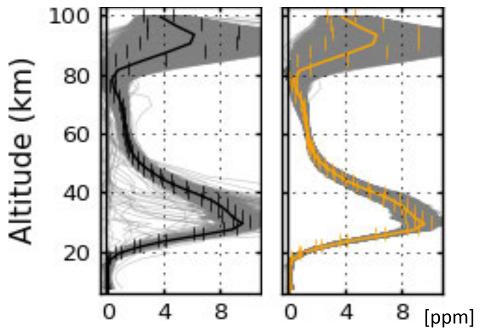
V2.3: Status flag updates

Ratios of useful data (status flag = 0)

	A	B	C
V2.2	63.0	62.2	29.3
V2.3	94.2	93.9	81.6

Screening example (O3, bandA, S10-N10)



- **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 .**

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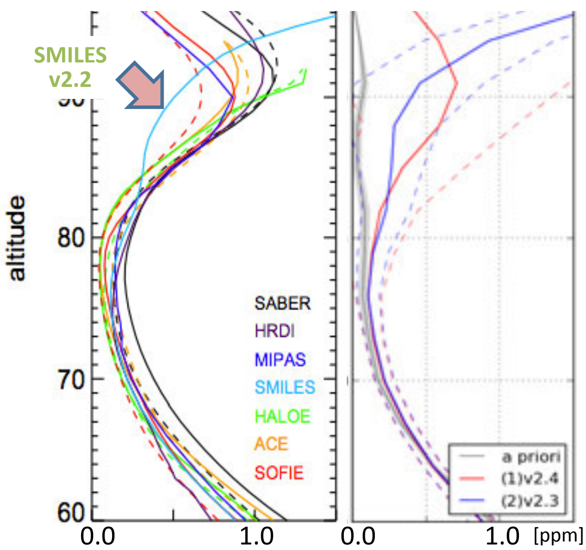
V2.4: mesosphere profile updates

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.

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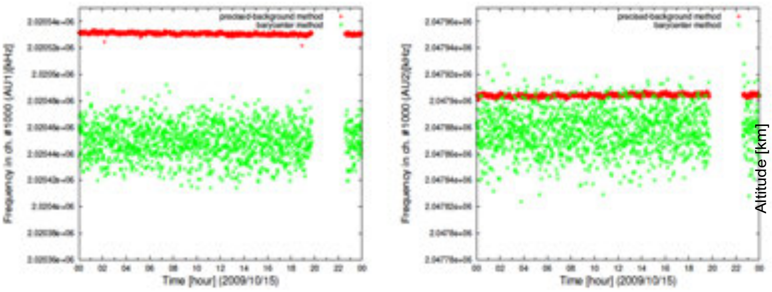
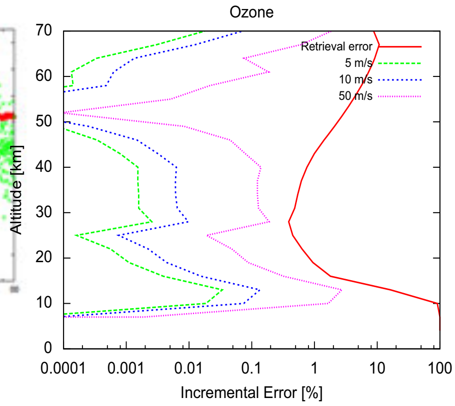
v2.4: Impact of L1B v008, Frequency Calibration.





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.

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.

v1.0-2.4: Spectroscopy

O_3 and O_3 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

Parameters	L2 v1.3	v2.0	Reference
O_3			
- γ_0 (MHz/hPa)	624371.112	624371.223	Ozeki private communication (preliminary results)
- n_γ			
	2.258	2.3078	HITRAN2008
	0.77	0.78	HITRAN2008
$H^{35}Cl$			
- Line position (MHz)	625901.603	625901.6584	Colmont et al., 2005
	625918.756	625918.6975	
	625932.007	625932.0081	
- γ_0 (MHz/hPa)	2.57	2.541	MLS Forward model ATBD (v1.0)
- n_γ	0.73	0.723	MLS Forward model ATBD (v1.0)
$H^{37}Cl$			
- Line position (MHz)	624964.374	624964.3694	Colmont et al., 2005
	624977.821	624977.8013	
	624988.334	624988.2821	
- γ_0 (MHz/hPa)	2.57	2.541	MLS Forward model ATBD (v1.0)
- n_γ	0.73	0.723	MLS Forward model ATBD (v1.0)
ClO			
- Line position (MHz)	649445.040	649445.250	Oh and Cohen, 1994
	649451.170	649451.072	
^{18}OOO			
- Line position (MHz)	649137.611	649137.132	Ozeki private communication (preliminary results)
	649137.611	649137.132	
	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_2.
- Future works.
  - Baseline issue caused by the AOS characteristics (over power RF inputs).
  - Gamma-air, temperature exponent (n), pressure shift.
  - any other ...

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

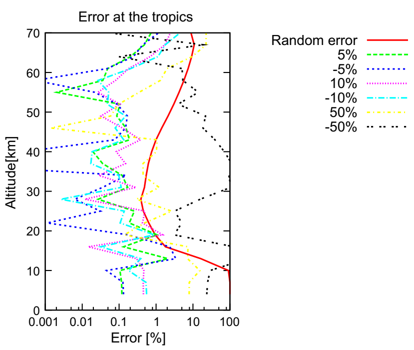
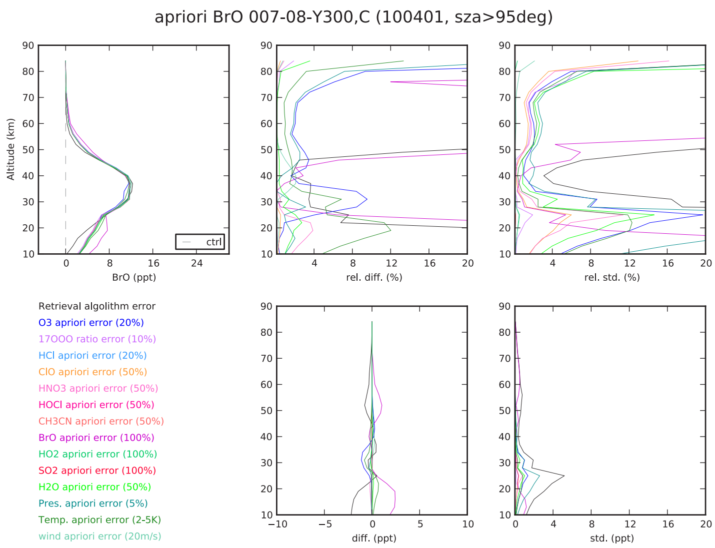


Fig. 5. Estimations for the influence of priori profiles in O_3 retrieval (in this case, a priori profiles are same as initial profiles). The solid red line is the random error of O_3. The other lines are additional errors between the true profiles of O_3 and the retrieved profiles of O_3 that are the final results of the iteration process in the cases where the differences between the a priori profiles and true profiles are ±5%, ±10%, and ±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.)



O_3 a priori impacts to O_3.
Takahashi, Suzuki et al. 2011

L2 v2.0: a priori impact to Band C BrO.
O3 and BrO have significant impact.
(unpublished internal work)

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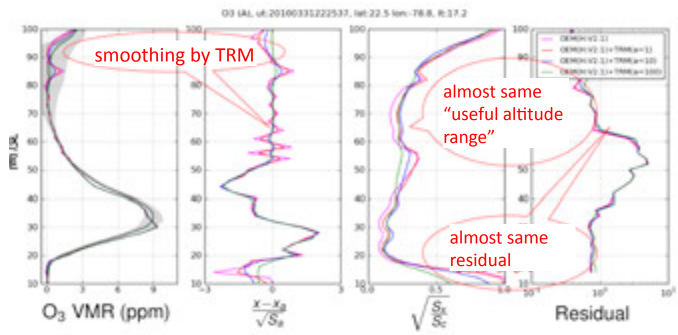
V3.0: Tikhonov regularization (TRM) to other species.

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, HCl, and HNO3)
Tikhonov L_1 was used, $L_1 + L_2$ method may be applied in future.

ハイブリッド法（OEM+TRM）

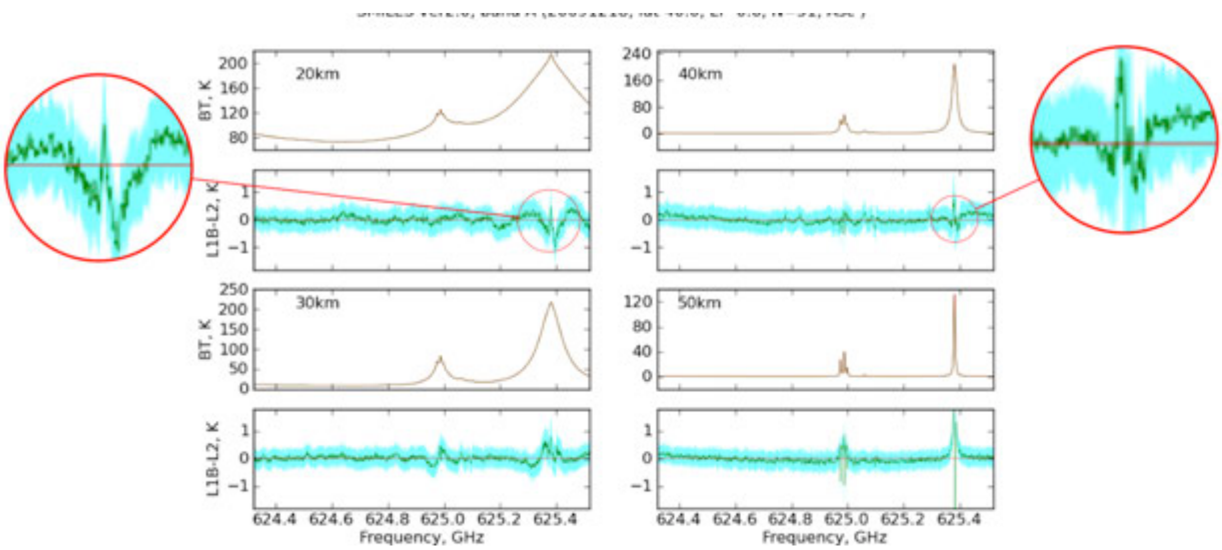
$$C_{hyb}(\mathbf{x}) = (\mathbf{x}-\mathbf{x}_a)^T \mathbf{S}_a^{-1} (\mathbf{x}-\mathbf{x}_a) + (\mathbf{x}-\mathbf{x}_a)^T \mathbf{L}^T \mathbf{S}_r^{-1} \mathbf{L} (\mathbf{x}-\mathbf{x}_a)$$

$\mathbf{S}_r \cdots$ “variance-covariance matrix” of regularization



- Similar result can be obtained with HCl and HNO3

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))

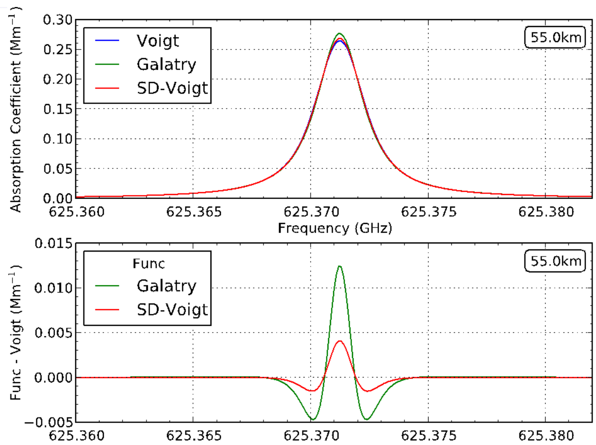
$$\varphi = \exp\left(ix_0 t - \gamma t - \frac{\sigma^2 t^2}{2}\right)$$

- Galatry Function
  - Dicke narrowing

$$\varphi = \exp\left(ix_0 t - \gamma t - \frac{\sigma^2(1 - \beta t - \exp(-\beta t))}{\beta^2}\right)$$

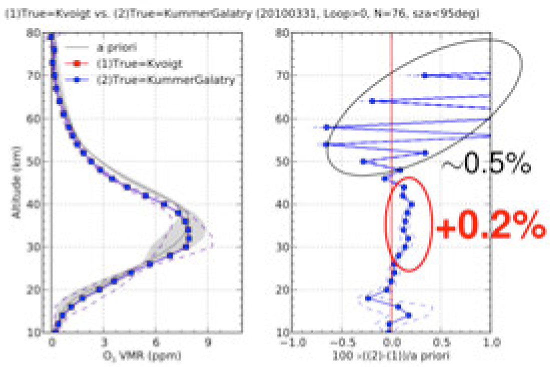
- Speed-dependent Voigt Function
  - Considering speed-dependence of collision width

$$\varphi = \frac{\exp\left(ix_0 t - (\gamma - 1.5\gamma_2 t) - \frac{\sigma^2 t^2}{2(1+\gamma_2 t)}\right)}{(1+\gamma_2 t)^{1.5}}$$

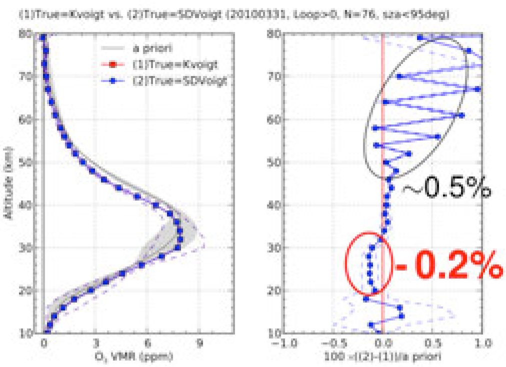


Galatry and SD-Voigt, impacts to O_3 retrieval are small but different. High altitude (> 50 km) systematic difference from Voigt function may exist.

- Galatry



- SD-Voigt



- 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	Galatry		SD-Voigt	
O_3 (day)	A	+0.2%	30~40km	−0.2%	20~30km
O_3 (day)	B	−0.2%	10~20km	−0.2%	20~30km
O_3 (day)	A	+0.5%	50~80km	+0.5%	50~80km
O_3 (day)	B	+0.5%	50~80km	+0.3%	50~80km
O_3 (night)	A	+0.2%	30~40km	−0.3%	20~30km
O_3 (night)	B	−0.2%	15~25km	−0.3%	20~30km
O_3 (night)	A	+0.5%	50~80km	+0.3%	50~80km
O_3 (night)	B	+0.4%	50~80km	+0.2%	50~80km
HCl	A	−0.3%	15~25km	-0.8%	15~25km
HCl	B	−0.2%	15~20km	-0.4%	15~20km
Temperature	A,B	−0.1K	20~40km	+0.1K	20~40km
HOCl (day)	A	+1%	30~40km	−1%	30~40km
HOCl (night)	A	+2%	30~40km	−3%	30~40km
CH_3CN	A	+3%	10~40km	+6%	10~30km

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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.**

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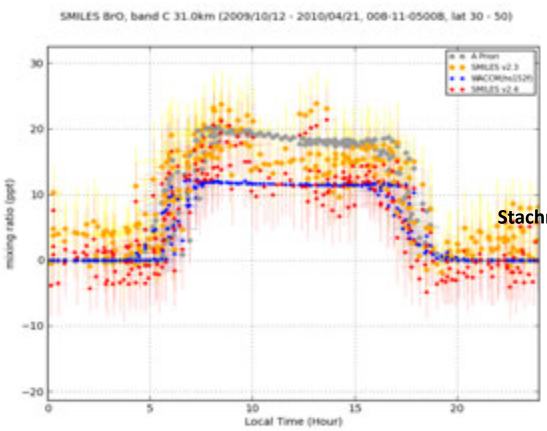
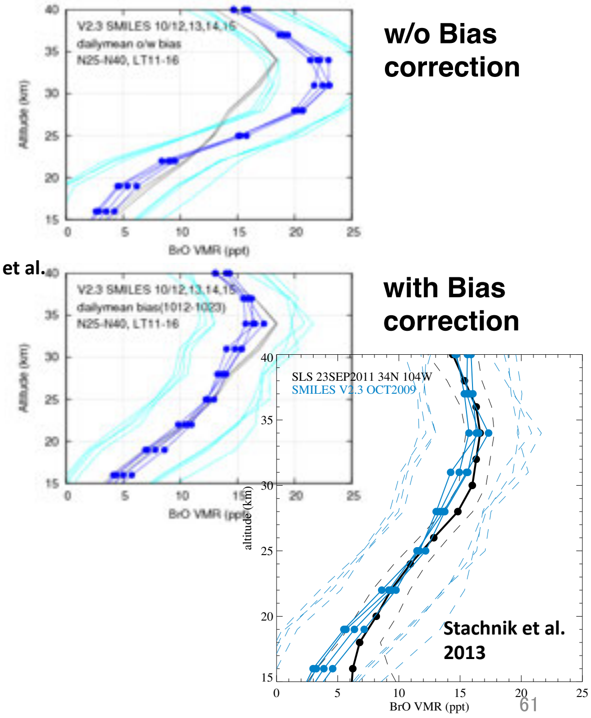
V3.0: Bias correction information for BrO, ClO, HO_2.



Stachnik et al.



w/o Bias correction

with Bias correction

BrO Diurnal variation revealed large night time bias.
Bias changed versions to versions.
Bias changed among latitude bins (and probably seasonally).

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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.

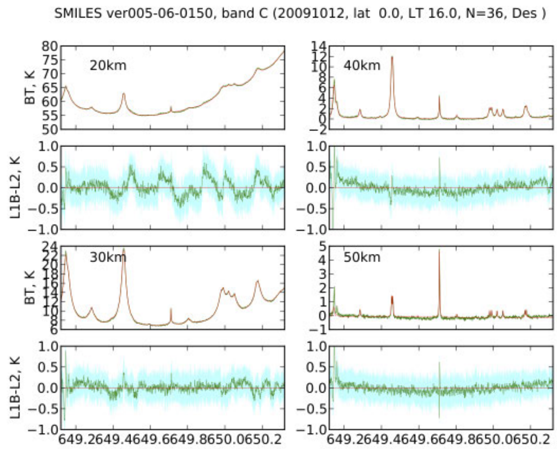

Fig. 6. Averaged spectra and residual spectrum (green: L1B, brown: L2 forward model calculation) of Band C on Oct. 12, 2009 at the equatorial region (±5°), descending orbit, for the tangent height 20 km (upper left), 30 km (lower left), 40 km (upper right) and 50 km (lower right); Number of sample is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

Suzuki et al. 2012

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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.

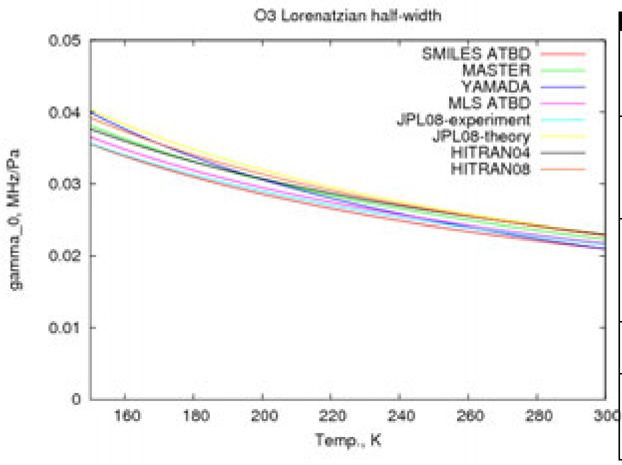

Table 5 updated line parameters

Parameters	L2 v1.3	v2.0	Reference
O_3			
- γ_0 (MHz/hPa)	624371.112	624371.223	Ozeki private communication
- n_γ			(preliminary results)
	2.258	2.3078	HITRAN2008
	0.77	0.78	HITRAN2008
$H^{35}Cl$			
- Line position (MHz)	625901.603 625918.756 625932.007	625901.6584 625918.6975 625932.0081	Colmont et al., 2005
- γ_0 (MHz/hPa)	2.57	2.541	MLS Forward model ATBD (v1.0)
- n_γ	0.73	0.723	MLS Forward model ATBD (v1.0)
$H^{37}Cl$			
- Line position (MHz)	624964.374 624977.821 624988.334	624964.3694 624977.8013 624988.2821	Colmont et al., 2005
- γ_0 (MHz/hPa)	2.57	2.541	MLS Forward model ATBD (v1.0)
- n_γ	0.73	0.723	MLS Forward model ATBD (v1.0)
ClO			
- Line position (MHz)	649445.040 649451.170	649445.250 649451.072	Oh and Cohen, 1994
^{18}OOO			
- Line position (MHz)	649137.611 649137.611 649149.603 649152.601	649137.132 649137.132 649152.038 649152.038	Ozeki private communication (preliminary results)

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.

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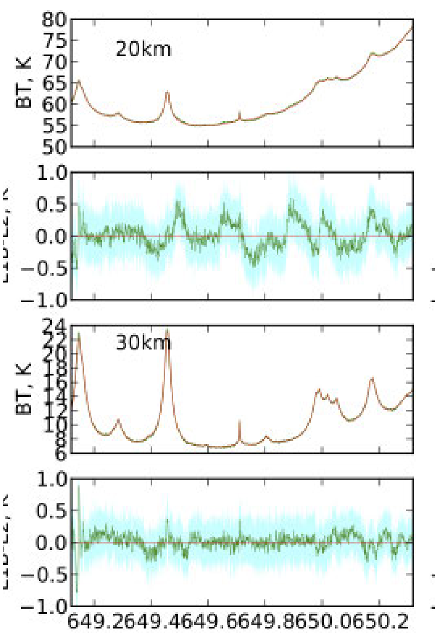
Future: Pressure Shift (1/2)

- **From v1.0 to v2.4, we considered pressure shift of O_3 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.**



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Future: Pressure Shift (2/2)

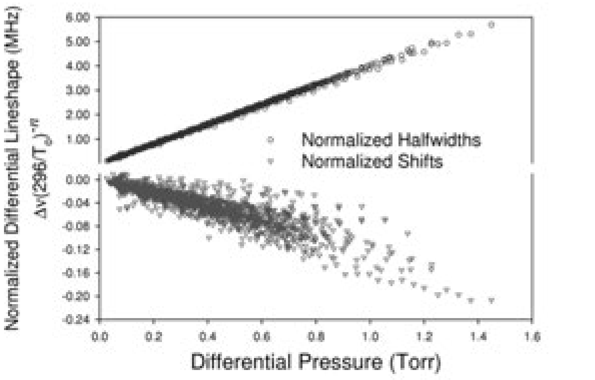

Figure 3. Broadening and shift measurements of HOCl $^rQ_0$-branch transitions near 630 GHz.

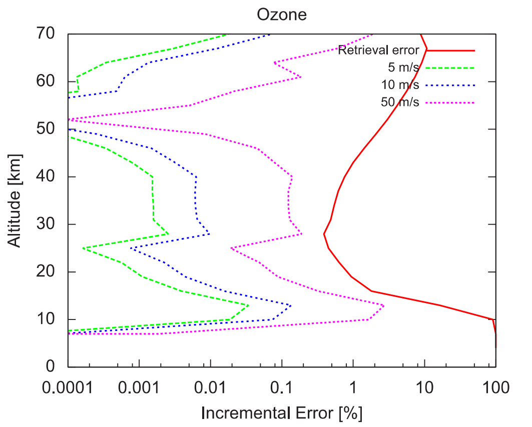

Fig.3. Effect of Wind. The red (solid) line indicates the retrieval precision of ozone. The other lines indicate the error due to the difference between the reference profile and the true profile of wind. (The wind velocities for the pink (fine dotted), blue (dotted), and green (dashed) profiles are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

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

50 m/s == 104 kHz.

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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.**

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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. Millán, R. Jarnot, R. Monroe, C. McLinden, S. Kühl, J. Pukīte, 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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- **We appreciate these teams to provide comparison data.**
  - **Satellite mission :**
    - **Aura/MLS, UARS/MLS, TIMED/SABER**
  - **Meteorology/Model :**
    - **GEOS5, WACCM, CCSR/NIES**

- **Thank you for your attention!**

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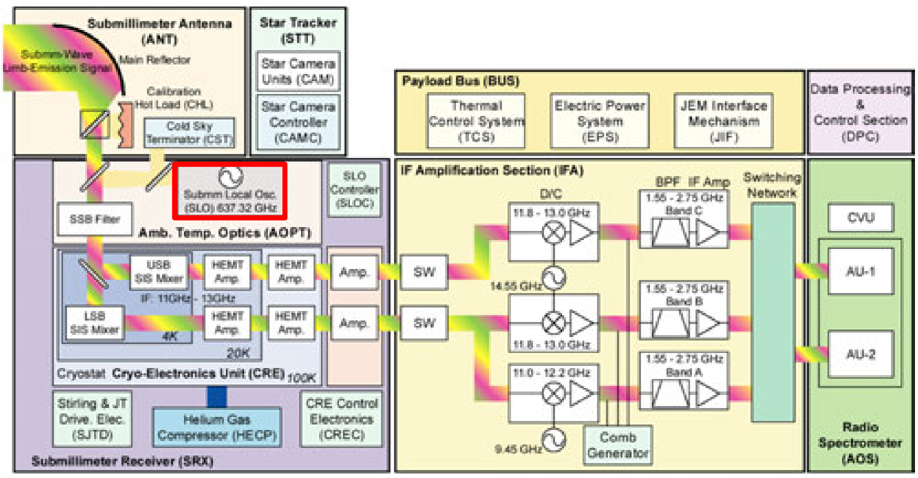
Summary of SMILES instrumental troubles in JAXA

29 March 2013

Institute of Space and Astronautical Science (ISAS),
Japan Aerospace Exploration Agency (JAXA)

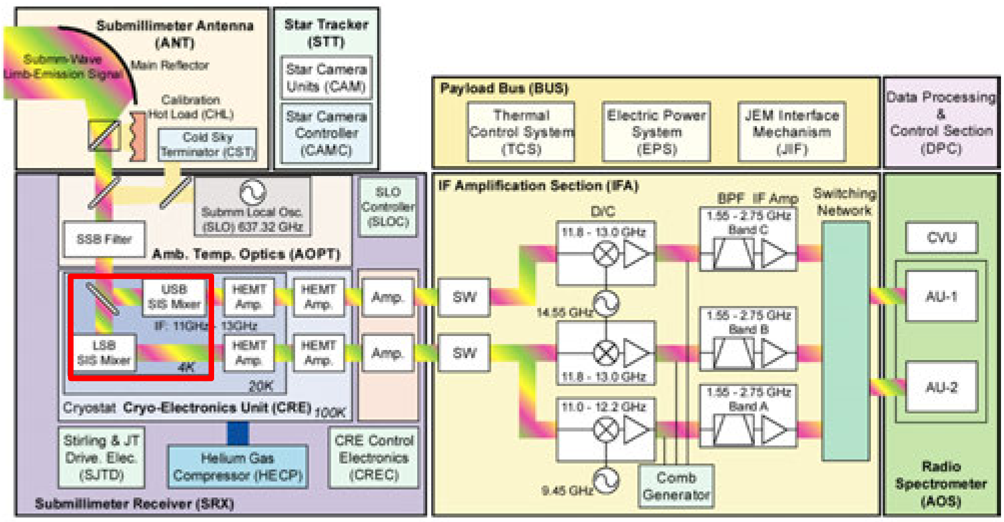
(1) Sub-mm Local Oscillator Failure



(1) Sub-mm Local Oscillator Failure

- SLO failure resulted in discontinuation of atmospheric observation directly. (Apr. 2010)
- A task force for SLO failure had been organized inside NICT*
  - NICT was in charge of development of SLO component
- SLO failure is caused by an occasional breakdown of Gunn diode.
  → Low reliability of Gunn diode (COTS)
- Lessons learned for future missions: redundant design is necessary for such component using COTS
- NICT task force reported this conclusion to the Space Activities Commission in Japanese government. (Jan. 2011)

(2) Restart Trouble of the Cryocooler

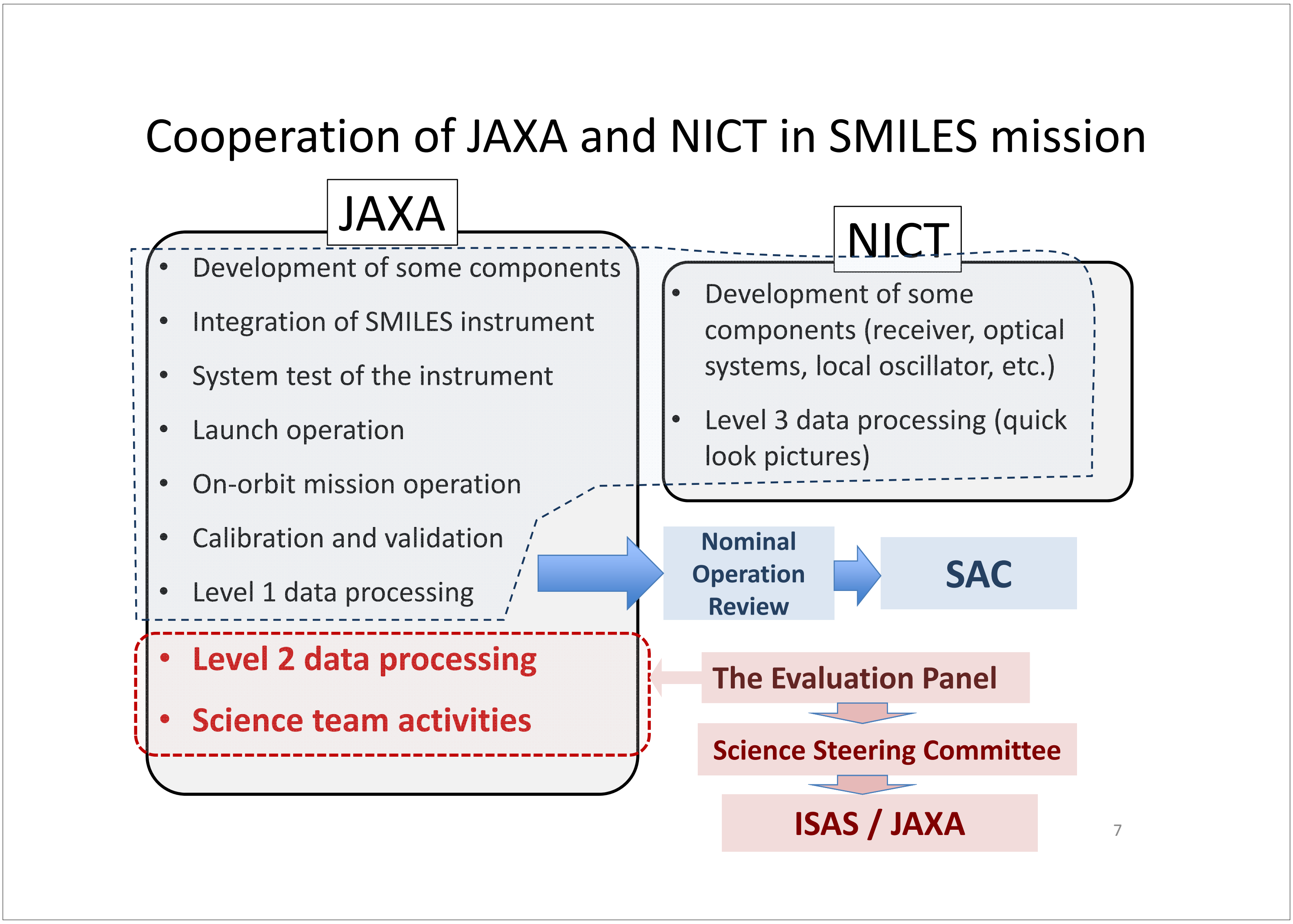


(2) Restart Trouble of the Cryocooler

- After JEM thermal control trouble, SMILES' cryocooler would not get back to 4K cooling mode. (June 2010)
- A task force of cryocooler developers worked on failure analysis, including additional ground experiment.
- Cryocooler trouble is caused by increased contamination gas (CO2) to helium gas in 4K cryocooler fluid system.
  → CO2 gas may came from compressor components.
- The lessons learned from this trouble is utilized to the development of cryocooler onboard coming astronomy satellite; control of baked materials, additional getter to cryocooler fluid system.
- The task force discussed this conclusion with "safety and reliability" teams in JAXA, and then reported them to the Space Activities Commission in Japanese government. (Jan. 2011)

Space Activities Commission in Japan

- SAC summarized the performance of SMILES instruments including on-orbit trouble and its failure analysis
- SAC approved the achievement of SMILES' success criteria
- SAC recommended the 3-year data processing, algorithm improvement, and scientific analysis
- SAC decided to terminate SMILES on-orbit "nominal operation"


Cooperation of JAXA and NICT in SMILES mission
JAXA
• Development of some components
• Integration of SMILES instrument
• System test of the instrument
• Launch operation
• On-orbit mission operation
• Calibration and validation
• Level 1 data processing
• Level 2 data processing
• Science team activities
NICT
• Development of some components (receiver, optical systems, local oscillator, etc.)
• Level 3 data processing (quick look pictures)
Nominal Operation Review
SAC
The Evaluation Panel
Science Steering Committee
ISAS / JAXA
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Japan Aerospace Exploration Agency