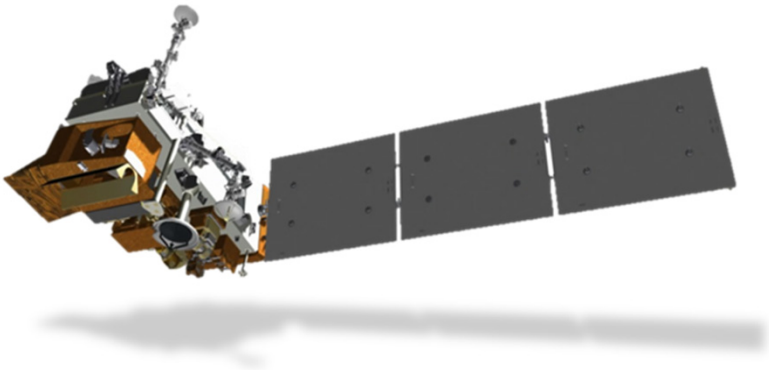
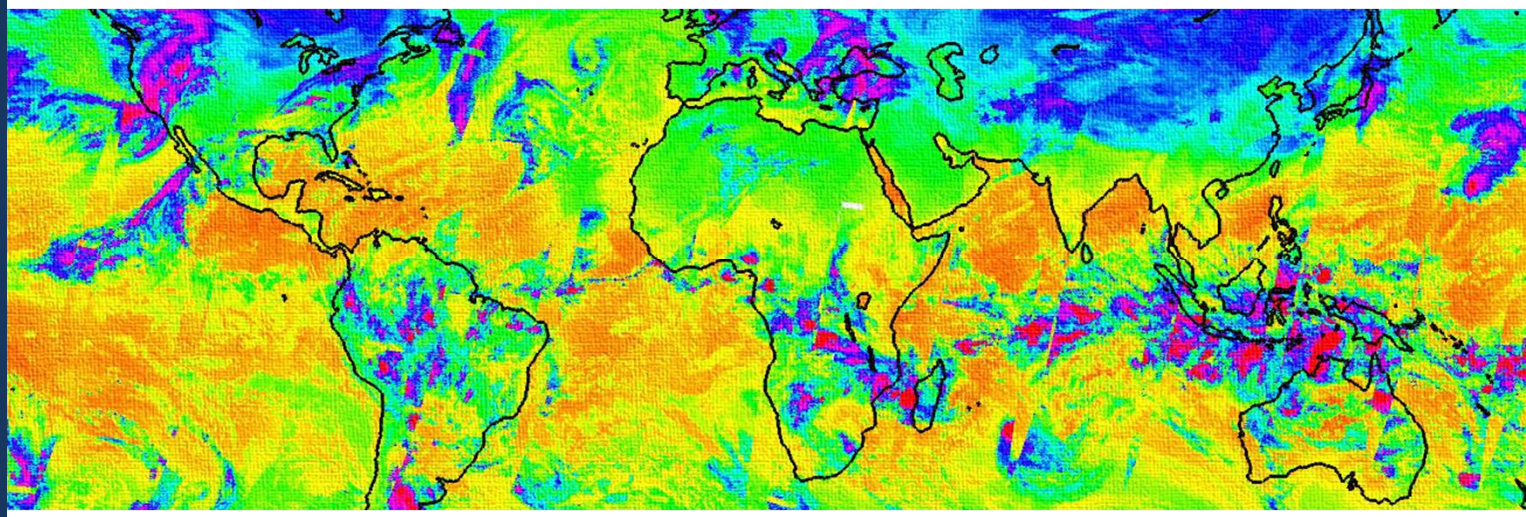
Advancing Atmospheric Chemistry Through the Use of Satellite Observations from the Cross-track Infrared Sounder (CrIS)

CrIS Atmospheric Chemistry Data User's Workshop Report
Sept. 18-19, 2014. College Park, MD.





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1 Executive Summary

The scientific communities studying atmospheric chemistry and its effects on air quality and climate change extensively use trace gas retrievals from thermal infrared (TIR) satellite observations. These products have been provided by NASA Earth Observing System (EOS) instruments, such as the Tropospheric Emission Spectrometer (TES), the Atmospheric Infrared Sounder (AIRS), and the Measurements of Pollution In The Troposphere (MOPITT) instruments, as well as by the Infrared Atmospheric Sounding Interferometer (IASI) aboard the EUMETSAT MetOp satellites. However, all of the EOS TIR sounders are currently well past their expected design lifetimes, and NASA does not have current plans to replace these instruments. This places critical data products at risk. The loss of these products would substantially harm key scientific studies focused on air quality, climate change, and Earth system processes.

There is, however, a solution. The Cross-track Infrared Sounder (CrIS) instrument, a Fourier Transform Infrared (FTIR) spectrometer currently flying aboard the joint NOAA, NASA and DOD Suomi National Polar-orbiting Partnership (Suomi-NPP) satellite, has the potential to continue many of these trace gas data records. As CrIS will also be flown aboard the upcoming NOAA Joint Polar Satellite System (JPSS) satellites, it could continue to produce TIR trace gas retrievals throughout the coming decade and beyond.

The CrIS Atmospheric Chemistry Data Users Workshop, held at NOAA Center for Weather and Climate Prediction in College Park, MD, was designed to ensure that CrIS could reach its full potential as an atmospheric composition instrument. The goals of the workshop were to:

- Generate communication between the CrIS retrieval algorithm development community and the atmospheric chemistry user community;
- Identify users and applications of current and future retrievals;
- Ensure sufficient validation of retrieval products;
- Identify limitations of current products; and
- Identify potential new retrieval products.

The workshop generated extensive discussion between researchers on all of the above issues, and this report summarizes our major conclusions and recommendations on the use, validation, improvement, and expansion of the current CrIS trace gas retrieval product suite. More details on each conclusion and recommendation are provided in the noted sections of the full report.

1.1 Conclusions and Recommendations

Conclusion 1:

We find that the primary limitation of the operational CrIS trace gas product suite is the degraded spectral resolution of the mid-wave and short-wave bands. Full resolution raw data is now available from CrIS as of December 2014, but current processing plans do not include producing calibrated radiances at this resolution.

Recommendation 1:

Calibrated radiances (Level 1b) should be provided at the full CrIS spectral resolution for use in the retrieval of trace gases as soon as possible, and this product should also be provided for the CrIS sensors for all future JPSS missions.

Conclusion 2:

We find that there is an extensive community of research and operational users, including NOAA centers and NOAA-funded researchers, who (a) depend on TIR trace gas retrievals for their work and (b) want to and would be able to use CrIS trace gas retrievals in their work (see Section 3). However, the number of current users of operational CrIS trace gas retrieval products is small. We make the following recommendations to expand the use of CrIS trace gas retrieval products (see Section 6):

Recommendation 2a:

The National Environmental Satellite, Data, and Information Service (NESDIS) should provide reduced files, modeled on the TES "lite" products that provide the retrievals for individual trace gases and their observation operators at a reduced vertical resolution. These would be in addition to the granule files provided at the full vertical resolution of the CrIS forward radiative transfer model through the Comprehensive Large Array-data Stewardship System (CLASS).

Recommendation 2b:

The reduced product files from Recommendation 2a need to provide a means to build an observation operator for each retrieval. This should include the averaging kernel, the estimated retrieval error, and the *a priori* profile. This information is essential to using CrIS trace gas retrievals in atmospheric chemistry studies. We further recommend that the NESDIS and CLASS teams explore approaches to reducing the size of these files, for example using a singular value decomposition (SVD) approach.

Recommendation 2c:

The CLASS archive should be updated to support convenient and rapid multi-file download of the reduced product files.

Conclusion 3:

We find that the current state of validation of the NOAA Unique CrIS/ATMS Processing System (NUCAPS) trace gas retrievals is insufficient for the use of these retrievals in most atmospheric chemistry applications (see Section 5). We make the following recommendations to address this need:

Recommendation 3a:

The CrIS retrieval development community should closely coordinate with the project teams of upcoming field campaigns (aircraft, surface, balloon, etc.) on trace gas validation activities, including US-led as well as European and other non-US campaigns. This coordination should include (i) working with the flight planning teams, (ii) ensuring timely data access, and (iii) fielding remote sensing instruments to augment the campaigns.

Recommendation 3b:

More frequent NOAA Earth System Research Laboratory (ESRL) aircraft flights are needed for validation of trace gas retrievals from CrIS (as well as from other satellite observations) for both climate-relevant and air quality-relevant species, including flights designed to investigate apparent anomalies in the CrIS trace gas retrievals. Since CrIS is sensitive to different altitude ranges for different gases, fights of a variety of aircraft with different instrumentation and altitude ranges will be required to validate all of the trace gases retrieved by CrIS.

Recommendation 3c:

In addition to the above activities, additional field campaigns and validation activities should be performed to fully validate the CrIS trace gas products, including products from future JPSS missions. These campaigns should involve both the retrieval development and the product user community.

Recommendation 3d:

All validation data should be added to the NESDIS Validation Archive (VALAR) so that future CrIS retrieval algorithms can be more easily evaluated against these data sets.

Conclusion 4:

We find that CrIS can continue most of the NASA EOS TIR trace gas data records (e.g., CO, O_3, CH_4, CO_2, NH_3, N_2O, SO_2, HNO_3, CH_3OH; see Sections 4 and 7.1), with the key exceptions of formic acid (HCOOH) and peroxyacetyl nitrate (PAN), which fall in the CrIS spectral gaps. In addition, the remarkably low noise of CrIS opens the possibility for several new trace gas retrieval products (see Section 7.2), including important species such as ethane (C_2H_6), acetylene (C_2H_2), ethylene (C_2H_4), hydrogen cyanide (HCN), and acetic acid (CH_3COOH).

Recommendation 4a:

We recommend that the CrIS retrieval community explore the development and validation of retrievals for the potential new species in close coordination with atmospheric chemistry research users who desire these products.

Recommendation 4b:

We recommend that the current spectral gap between the long-wave and mid-wave bands of CrIS be closed for JPSS-2, allowing the continuation of the EOS trace gas data records for HCOOH and PAN. We note that closing these spectral gaps was also a recommendation of the "JPSS 2 and Beyond: Instrument Improvements for Science Benefits" Workshop held on October 23, 2014.

Recommendation 4c:

We recommend that for post-JPSS planning, NOAA continue the polar-orbiting IR sounder program, and that NOAA consider approaches to both reduce the noise and increase the resolution of future versions of CrIS, as is being done in the New Generation of Infrared Atmospheric Sounding Interferometer (IASI-NG) program.

2 Introduction

The CrIS Atmospheric Chemistry Data Users Workshop was organized to identify current and potential uses of satellite observations from the CrIS in both research and operational applications focused on atmospheric composition and its impacts on air quality and climate. The scientific communities studying atmospheric chemistry, air quality, carbon cycle, nitrogen cycle, and climate change extensively use trace gas retrievals from TIR satellite observations [e.g., *Zhang et al.*, 2006; *Logan et al.*, 2008; *Jones et al.,* 2009; *Bowman et al.*, 2009; *Pierce et al.,* 2009, *McMillan et al.,* 2010, *Kopacz et al.,* 2010; *Heald et al.,* 2012; *Wecht et al.,* 2012; *Wells et al.*, 2012, 2014; *Crevoisier et al.*, 2013; *Worden, J. et al.*, 2013a,b; *Zhu et al.,* 2013; *Cady-Pereira et al.,* 2012, 2014; *Stavrakou et al.,* 2011, 2012]. These products have been provided by NASA EOS instruments, such as TES, AIRS, and MOPITT, as well as IASI aboard the EUMETSAT MetOp satellites. However, all of the EOS TIR sounders are currently well past their expected design lifetimes, and NASA does not have current plans to replace these instruments. This places critical data products at risk. The loss of such products would substantially harm key scientific studies focused on air quality, climate change, and Earth system processes.

However, the CrIS instrument, a FTIR spectrometer currently flying on board the Suomi-NPP satellite, has the capability to continue many of these data records for gases such as CO, O_3, CH_4, CO_2, N_2O, HNO_3, CH_3OH, and NH_3 [*Strow et al.,* 2013; *Bowman et al.,* 2011]. CrIS can provide soundings of the atmosphere in three bands (long-wave between 650 – 1095 cm^{-1}, mid-wave between 1210 – 1750 cm^{-1}, and short-wave between 2155 – 2550 cm^{-1}) at a spectral resolution of 0.625 cm^{-1}. CrIS scans a 2200 km swath width (+/- 50 degrees) with an array of circular pixels of 14 km diameter each (nadir spatial resolution). The large swath and small pixel size of CrIS allow it to provide atmospheric retrievals globally twice a day (~1:30 AM/PM local solar time).

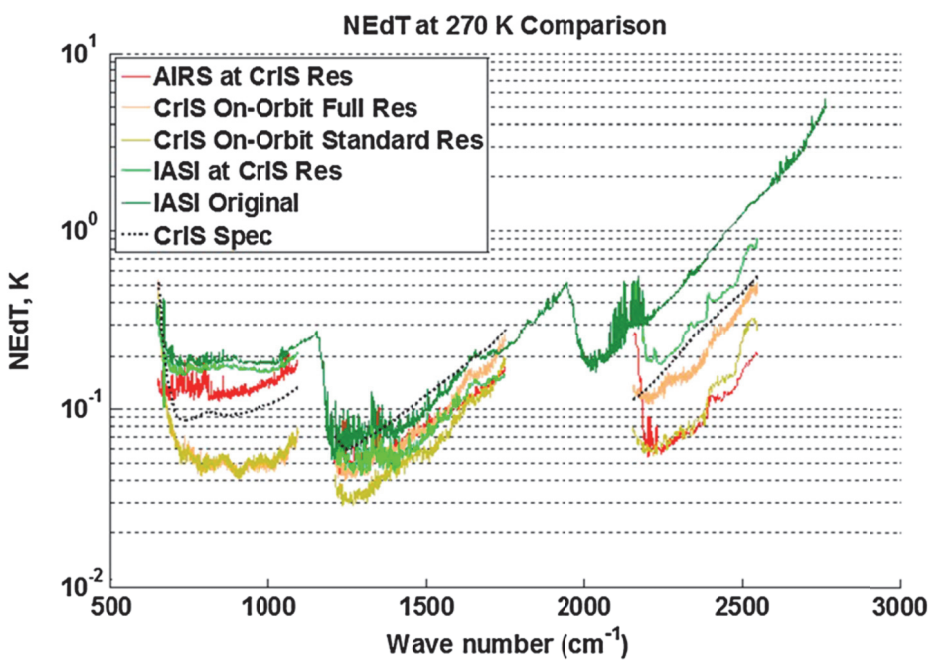

Figure 1. CrIS noise-equivalent brightness temperature difference (NEdT, K) as compared to IASI and AIRS. Figure reproduced from Zavyalov et al. [2013].

Current operational CrIS measurements have degraded the CrIS spectral resolution in the mid-wave and short-wave bands (a factor of 2 and 4, respectively, compared to the long-wave band) so as to reduce the amount of data processed by the ground stations. Plans to increase the mid-wave and short-wave spectral resolution to match the long-wave spectral resolution are being implemented and full resolution raw CrIS data became operational in December 2014. The full CrIS spectral resolution is better than AIRS and comparable to IASI, and the spatial coverage is superior to that of TES. Its equatorial crossing times (~1:30 AM and 1:30 PM) are very close to those of AIRS and TES; the daytime crossing time is optimal for retrieving species with high concentrations near the surface, as these retrievals work best when the thermal contrast between the surface and the target species is high. CrIS has a significantly higher signal to noise ratio (SNR) than TES, IASI or AIRS (Figure 1); this high SNR can partially compensate for a poorer spectral resolution compared to TES.

As CrIS will also be flown aboard the upcoming NOAA JPSS satellites, it has the potential to continue to produce TIR trace gas retrievals throughout the coming decade and beyond. However, there are currently several limitations preventing the use of CrIS trace gas products by the atmospheric science and operational application end users. First, there is a need for better communication and collaboration between the CrIS retrieval communities and the potential end users of the trace gas retrieval products. Second, there is a need for a coordinated strategy to validate trace gas products from CrIS and to identify any needed changes to the current CrIS trace gas products to facilitate their use by scientific and operational end users.

The CrIS Atmospheric Chemistry Data Users Workshop addressed these needs by bringing together the retrieval algorithm, scientific, and operational communities working with TIR trace gas retrievals (see Table 1) to develop a strategic plan for the development, validation, dissemination, and use of CrIS trace gas products. The goals of the workshop were to:

- Generate communication between the CrIS retrieval algorithm development community and the atmospheric chemistry user community;
- Identify users and applications of current and future retrievals;
- Ensure sufficient validation of retrieval products;
- Identify limitations of current products; and
- Identify potential new retrieval products.

This community report summarizes the findings and recommendations of the workshop. Section 3 lists current and potential research and operational users of trace gas retrieval products from CrIS. Section 4 summarizes the status of the current CrIS retrieval products. Section 5 describes the validation needs for these products and discusses current data sources and planned measurement campaigns that can address these needs. Section 6 describes changes that need to be made to the CrIS retrieval product files, including suggestions for reducing file size and facilitating the use of the data. Section 7 then discusses potential new products that may be able to be retrieved given the remarkably low noise of CrIS, and two products (HCOOH and PAN) that could be retrieved if the spectral gap between the long-wave and mid-wave CrIS bands were removed for JPSS-2 and beyond.

Table 1. Workshop Attendees

	Name	Institution
Extramural		
1	Alvarado, Matthew (Chair)	Atmospheric and Environmental Research, Inc.
2	Barnet, Chris	Science and Technology Corporation
3	Bowman, Kevin	NASA Jet Propulsion Laboratory
4	Jones, Dylan	University of Toronto
5	Merrelli, Aronne	University of Wisconsin SSEC/CIMSS
6	Millet, Dylan	University of Minnesota
7	Nowak, John	Aerodyne Research, Inc.
8	Saikawa, Eri	Emory University
9	Smith, Nadia	University of Wisconsin SSEC/CIMSS
10	Warner, Juying	University of Maryland
11	Worden, Helen	National Center for Atmospheric Research
12	Yurganov, Leonid	University of Maryland Baltimore County Joint Center for Earth Systems Technology
13	Zhu, Liye (Juliet)	Colorado State University
NOAA OAR		
14	De Gouw, Joost	NOAA ESRL Chemical Sciences Division
15	Fahey, David	NOAA ESRL Chemical Sciences Division
16	Kim, Si-Wan	NOAA ESRL Chemical Sciences Division
17	Mao, Jingqiu	NOAA Geophysical Fluid Dynamics Laboratory
18	Neuman, Andrew	NOAA ESRL Chemical Sciences Division
19	Rosenlof, Karen	NOAA ESRL Chemical Sciences Division
20	Tong, Daniel	NOAA Air Resources Laboratory
NOAA/NESDIS		
21	Goldberg, Mitch	NOAA NESDIS Joint Polar Satellite System
22	Gambacorta, Antonia	NOAA NESDIS Center for Satellite Applications and Research (CSAR, College Park, MD)
23	Liu, Quanhua (Mark)	NOAA NESDIS CSAR (College Park, MD)
24	Nalli, Nicholas	NOAA NESDIS CSAR (College Park, MD)
25	Wolf, Walter	NOAA NESDIS CSAR (College Park, MD)
26	Xiong, Xiaozhen	NOAA NESDIS CSAR (College Park, MD)
27	Pierce, Bradley	NOAA NESDIS CSAR (Wisconsin)
28	Sharma, Awdhesh	NOAA NESDIS CSAR (College Park, MD)
Remote		
1	Andrews, Arlyn	NOAA ESRL Global Monitoring Division
2	Fischer, Emily	Colorado State University
3	Henze, Daven	University of Colorado, Boulder
4	Karion, Anna	NOAA ESRL Global Monitoring Division
5	Sweeney, Colm	NOAA ESRL Global Monitoring Division
6	Wang, Jun	University of Nebraska, Lincoln
NOAA CPO		
1	Kopacz, Monika	NOAA Climate Program Office
2	Mooney, Kenneth	NOAA Climate Program Office
3	Randazzo, Nina	NOAA Climate Program Office
4	Sagar, Amrith	NOAA Climate Program Office

3 Users and Applications of TIR Trace Gas Retrievals

Primary Authors: *Dylan Millet, Brad Pierce, Dylan Jones, Kevin Bowman, Jingqiu Mao, Arlyn Andrews, Eri Saikawa, Chris Barnet, Shawn Xiong, Juying Warner, Emily Fischer, Juliet Zhu*

Potential uses for CrIS trace gas data include source attribution studies and trend analyses to quantify budgets of key climate and air quality gases, as well as data assimilation studies to improve emission estimates and forecasts of air quality and climate impacts. As we highlight below, TIR trace gas retrievals from instruments such as MOPITT, AIRS, TES, and IASI have provided powerful, global information for understanding atmospheric composition, air quality, and climate. With the exception of the second IASI instrument on MetOp-B, all of these instruments are well past their design lifetime. Developing similar data products from CrIS is thus a critical aspect of the global observing network that is needed to advance present knowledge of the atmosphere-climate system.

Below we divide our discussion into greenhouse gas retrieval products (e.g., CO_2, CH_4, O_3, and N_2O) and air quality retrieval products (e.g., CO, O_3, SO_2, NH_3, and CH_4). Note that there are several species, most notably O_3 and CH_4, that have important implications for both climate and air quality.

3.1 Greenhouse Gases

3.1.1 Operational

There are two separate potential operational uses for CrIS retrievals of greenhouse gases. The first is to use the retrieved greenhouse gas concentrations of O_3, CO_2, CH_4, and N_2O in chemical data assimilation into operational weather, carbon cycle, and climate models, such as is done by the EU Monitoring Atmospheric Composition and Climate (MACC-III) project [https://www.gmes-atmosphere.eu/about/project/macc_input_data/] for IASI retrievals of CO, CO_2 and CH_4. The second potential operational use is in the radiation scheme of numerical weather prediction and other models prior to assimilation of CrIS radiances.

It is appropriate to differentiate between "operational" and "real-time" applications for cases when data latency is important. Real-time availability and display of trace gas observations can be important in monitoring applications, such as disaster tracking or in field campaigns. The need for real-time observational data is recognized in the University of Wisconsin-Madison (UW) Community Satellite Processing Package (CSPP), which is funded by NOAA to prepare and release a direct-broadcast version of the NUCAPS software (and other science algorithms, such as the UW Dual-Regression algorithm) to the international community so that they may run this on their own local systems as data are received through antennae.

3.1.2 Research

The primary research use of greenhouse gas retrievals is in data assimilation and source attribution studies to establish constraints on the changing sources and sinks of atmospheric CO_2, CH_4, and N_2O. This research is being carried on by a large number of research groups worldwide; rather than attempt to present an exhaustive list of these efforts, here we focus on a few key examples of research efforts led by federal laboratories at NOAA and NASA, as well as related research efforts led by the participants in the CrIS workshop.

Dr. Vaishali Naik of the NOAA Geophysical Fluid Dynamics Laboratory (GFDL) is working on improving the representation of CH4 within the GFDL AM3 global model and applying this model to analyze the long-term trends and variability in atmospheric CH4 concentrations.

CrIS CH4 observations would provide constraints on source estimates as implemented in AM3. The extended TIR CrIS record would also assist in the investigation of long-term trends and variability in CH4.

The NASA CMS-Flux Project, led by Dr. Kevin Bowman from NASA JPL, depends on thermal IR CO2 measurements from satellites, along with other observations, to attribute changes in the atmospheric growth rate of CO2 to spatially explicit fluxes across the entire carbon cycle [Liu et al., 2014]. Furthermore, Dr. Bowman has pioneered the development and exploitation of observed outgoing long-wave radiation products from Aura TES and their sensitivity to tropospheric ozone to evaluate chemistry-climate models [Worden, H. M. et al., 2008; Aghedo et al., 2011; Bowman et al., 2013; Shindell et al., 2013a,b; Young et al., 2013] and attribute ozone radiative forcing to spatially-resolved emissions [Bowman and Henze, 2012]. CrIS could be used to extend this work.

Prof. Dylan Millet of the University of Minnesota is applying global surface and airborne observations in an adjoint modeling framework to establish new constraints on the surface emissions and stratospheric loss of atmospheric N2O as part of a NOAA CPO funded project. This and related projects would benefit significantly from robust space-based measurements in assessing the impact of stratosphere-troposphere exchange on atmospheric N2O.

Prof. Eri Saikawa of Emory University is working on a NOAA CPO funded project to assess what drives the seasonal and inter-annual variability of N2O emissions and the atmospheric mixing ratio of N2O. This project would also benefit from CrIS TIR observations of N2O.

Prof. Dylan Jones of the University of Toronto has used retrievals of CO2 from the TIR TES instrument to constrain surface fluxes of CO2 [Nassar et al., 2011]). He has found that the information on free tropospheric CO2 provided by TIR sounders provides additional constraints beyond the surface observation network, and that these can be particularly useful in improving features such as the CO2 distribution in the Asian monsoon region.

Dr. Juying Warner of the University of Maryland-Baltimore County (UMBC) uses AIRS observations of CH4 to investigate the sources and distribution of this gas in the atmosphere. Continuing the AIRS CH4 record with CrIS would substantially strengthen research efforts aimed at understanding the inter-annual variability of this gas.

3.2 Air Quality

3.2.1 Operational

The key potential operational air quality use for CrIS trace gas retrievals is near-real-time air quality and chemical weather forecasting. Such work is carried out by a diverse group of users both within and outside the US. Outside the US, the Composition component of the European Center for Medium-range Weather Forecasting (ECMWF) Integrated Forecasting System (C-IFS) represents the current state of the science with regard to global air quality assimilation and forecasting. C-IFS has fully integrated chemistry, aerosol, and greenhouse gas predictions; it assimilates atmospheric composition observations to simulate global atmospheric chemistry, including feedbacks between atmospheric composition and weather [*Flemming et al.,* 2013]. C-IFS currently assimilates IASI CO and O_3 retrievals. Likewise, Environment Canada provides operational air quality forecasts using the Global Environmental Multi-scale - Modeling Air quality and CHemistry (GEM-MACH) forecast system, which is run over North America to provide guidance for Canadian air quality forecasts. Testing of assimilation of surface air quality measurements has been conducted with the GEM-MACH system [*Robichaud and Ménard*, 2014].

In the US, the NOAA National Weather Service (NWS) and Air Resources Laboratory (ARL)

provide daily forecasts of surface ozone using the Community Multi-scale Air Quality (CMAQ) model driven with meteorology from the North American Model (NAM) through the National Air Quality Forecasting Capability. NAM-CMAQ assimilation experiments have been conducted to assess the impact of assimilating GOES Total Column Ozone retrievals within NAM-CMAQ [*Pierce et al.,* 2011], and similar assimilation of O_3 and CO products from CrIS could be used to improve the O_3 forecast. NOAA ARL is also developing a surface $PM_{2.5}$ forecasting system, and CrIS NH_3 observations will be extremely useful in constraining the highly uncertain emissions of this $PM_{2.5}$ precursor.

Other potential near-real-time CrIS air quality data users include:

- NOAA Global Forecast System (GFS)
- NASA Goddard Earth Observing System Model (GEOS-5)
- US Naval Research Laboratory Navy Operational Global Atmospheric Prediction System (NOGAPS)
- Various regional air quality forecasting organizations, for example at Georgia Tech., North Carolina, and Washington State.

In addition, near-real-time CrIS data could be useful in planning future aircraft sampling missions by providing information that allows the targeting of scientifically interesting locations.

3.2.2 Research

A number of research air quality modeling systems have conducted chemical data assimilation experiments using IR trace gas retrievals that are analogous to the CrIS products. IR trace gas assimilation studies have focused on assimilation of CO [*Lamarque et al.,* 1999] and the use of inverse modeling to constrain CO [*Kopacz et al.,* 2010], NH_3 [*Zhu et al.,* 2013] and CH_3OH [*Wells et al.,* 2014], as well as on joint O_3/CO assimilation [*Pierce et al.,* 2009] and adjoint emission constraint experiments [*Jones et al.,* 2009]. As above, rather than attempt an exhaustive list of users, we focus on efforts at federal laboratories and related research efforts by the workshop participants. Potential users of CrIS trace gas retrievals for air quality research and forecast system development include: NOAA ESRL, which focuses on pollution source analysis using the Weather Research and Forecasting with Chemistry model (WRF-Chem) and the Flexible Particle (FLEXPART) dispersion model, air pollution forecasts using the Rapid Refresh with chemistry (RR-Chem[1]) modeling system, and trend analysis of ozone and ozone precursors.

The UW-Madison/NESDIS Real-time Air Quality Modeling System (RAQMS[2]), which currently assimilates real-time O_3 retrievals from the NASA Ozone Monitoring Instrument (OMI) and the Microwave Limb Sounder (MLS) and will be used to assimilate AIRS CO, CH_4, and O_3 retrievals as part of a multi-sensor chemical reanalysis project.

The NOAA GFDL AM3 model development team is conducting on-going work on nitrogen cycling that would benefit from CrIS observations of NH_3, and could use CrIS retrievals of CO and O_3 to improve the spatial and temporal variability of these species in AM3. In particular, they plan to use CrIS for the upcoming NOAA field campaign FIREX[3] to better constrain biomass burning emissions and ozone production from biomass burning plumes.

The National Center for Atmospheric Research (NCAR), which currently assimilates IASI CO and O3 observations into Community Atmosphere Model with Chemistry (CAM-Chem) and WRF-Chem simulations, and also provides air quality forecasts using assimilation of MOPITT CO into the Model for OZone And

[1] http://ruc.noaa.gov/wrf/WG11_RT/

[2] http://raqms-ops.ssec.wisc.edu/index.php

[3] http://www.esrl.noaa.gov/csd/projects/firex/

Related chemical Tracers (MOZART-4) [Emmons et al., 2010]. In addition, Dr. Helen Worden of NCAR uses satellite observations to investigate the trends in CO, which have important implications for both air quality and climate. Continuing the record of CO measurements from MOPITT is critical for understanding the multi-decadal changes in CO [Worden, H.M. et al., 2013a].

The GEOS-Chem research community, which focuses on use of the adjoint of the Goddard Earth Observing System-Chemical transport model (GEOS-Chem) 4 for source inversion studies of multiple gases, such as CO [Kopacz et al., 2010], O3, and NH3 [Zhu et al., 2013].

Prof. Dylan Millet of the University of Minnesota, whose ongoing work employs TIR measurements of CH3OH (TES, IASI), HCOOH (TES, IASI) and CO (MOPITT) to better understand the sources and chemical impacts of these species and the constraints that these measurements can provide on the overall reactive carbon budget of the atmosphere [Cady-Pereira et al., 2012, 2014; Chaliyakunnel et al., 2013; Wells et al., 2012, 2014a,b].

Dr. Matthew Alvarado and Ms. Karen Cady-Pereira of AER, who are currently funded by NOAA CPO to use AER's CrIS NH3 retrieval to study the emissions of NH3 during the NOAA SENEX (SouthEast NEXus of climate change and air quality) campaign and over California in the summer of 2012.

Prof. Emily Fischer and Dr. Juliet Zhu of Colorado State University and Dr. Vivienne Payne of NASA JPL, who are using new PAN retrievals from TES [Payne et al., 2014] to investigate the role of fires in driving observed inter-annual variability of PAN at high latitudes, the relative importance of lightning versus fires in driving the austral spring PAN distribution, and the impact of PAN on the transpacific transport of O3.

Environment Canada, which utilizes TIR satellite measurements as part of their ongoing modeling and analysis efforts. This agency is interested in using CrIS measurements for chemical data assimilation to improve surface air quality analyses and forecasts as well as UV index forecasts, either directly or through synergy with other datasets. The retrieved CrIS constituent data (i.e. ozone) would contribute in the validation of the assimilation and forecasting products. In addition, Environment Canada's Dr. Mark Shephard and Dr. Chris McLinden are collaborating with AER to continue NH3 emission research over North America [Shephard and Cady-Pereira, 2014], including NH3 model validation.

[4] http://wiki.seas.harvard.edu/geos-chem/index.php/GEOS-Chem_Adjoint

4 Current CrIS Trace Gas Products

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Here we briefly describe two algorithms that are currently used or in development for the retrieval of trace gases from CrIS: the NUCAPS algorithm (Section 4.1) developed by NOAA NESDIS and the AER/NCAR retrievals of NH_3 and CO (Section 4.2).

4.1 Overview of NUCAPS

The NUCAPS algorithm currently retrieves the trace gases H_2O, O_3, CO, CO_2, CH_4, N_2O, HNO_3, and SO_2 from CrIS spectra [e.g., *Gambacorta and Barnet*, 2013] using 339 channels chosen based on their spectral properties, including spectral purity, independent information content, vertical sensitivity, low instrumental noise, and global optimality [*Gambacorta and Barnet*, 2013]. Table 2 shows the trace gases retrieved by the NUCAPS algorithm, along with the estimated precision, degrees of freedom for signal (DOFS, representing the number of independent pieces of information in the retrieved profile [*Rodgers*, 2000]), and the vertical region of maximum CrIS sensitivity for each gas. Note that the current, degraded resolution of the short-wave band (2.5 cm^{-1}) does not allow CrIS to provide meaningful information on CO [*Gambacorta et al.,* 2014], and thus the full-resolution (0.625 cm^{-1}) CrIS data are necessary for the optimal retrieval of CO, as well as for the retrievals of other gases that use channels in the mid-wave and short-wave bands (e.g., CH_4 and N_2O).

4.2 AER/NCAR CrIS Retrievals of NH_3 and CO

Ms. Karen Cady-Pereira of AER and Dr. Helen Worden of NCAR are leading an effort to develop operational optimal estimation CO and NH_3 retrievals from CrIS based upon the heritage from the TES and MOPITT retrieval algorithms. Atmospheric ammonia (NH_3) is the dominant base in the atmosphere. It plays key roles in atmospheric chemical processing: as an important source of $PM_{2.5}$ particles, it can significantly affect air quality, and deposition of this species can contribute to major changes in ecosystem health. The NH_3 retrievals from TES have been used in conjunction with the GEOS-Chem adjoint model to constrain NH_3 emissions [*Zhu et al.,* 2013]. TES NH_3 values are generally higher than initial model NH_3 distributions in the US and this indicates that NH_3 sources may be widely underestimated. NH_3 observations from CrIS provide a new opportunity for reducing persistent uncertainties of the distribution of atmospheric NH_3.

In addition, measurements of CO from space have been essential for understanding global atmospheric chemistry, transport, and emissions. Due to its medium-scale lifetime (weeks to months) CO is a useful tracer of pollution. It is transported globally but is not evenly mixed, allowing measurements of elevated CO that are easily distinguished above background levels. CO also serves as the reference gas for the emissions of many difficult-to-measure species, such as those co-emitted from combustion processes [*Luo et al.*, 2015].

The AER/NCAR retrieval algorithms for NH_3 and CO will use the same optimal estimation approach adopted for TES [*Bowman et al.,* 2006; *Shephard et al.*, 2011] and MOPITT [*Deeter et al.*, 2003; *Deeter et al.*, 2007], with similar microwindows and the same *a priori* vectors and constraint matrices, providing continuity with the TES and MOPITT databases. A prototype CrIS NH_3 algorithm has already been developed as part of a NOAA CPO project, and limited testing has shown good agreement with TES and surface observations. The high spatial and temporal coverage provided by CrIS is a significant advantage over TES [*Shephard and Cady-Pereira*, 2014].

Table 2. Spectral ranges, precision, and sensitivity of the NUCAPS retrievals of trace gases.

	Spectral Range (cm^{-1})	**Retrieval Precision**	**d.o.f.**	**Interfering Signals**	**Sensitivity**
H_2O	1200-1600	15%	4-6	CH_4, HNO_3	Surf. to 300 mb
O_3	1025-1050	10%	1+	H_2O, surface emissivity	Lower strat.
CO	2080-2200	15%	≈ 1	H_2O, N_2O	Mid-trop
CH_4	1250-1370	1.5%	≈ 1	H_2O, HNO_3, N_2O	Mid-trop
CO_2	680-795	0.5%	≈ 1	H_2O, O_3	Mid-trop
	2375-2395			T(p)	
Volcanic SO_2	1340-1380	50% ??	< 1	H_2O, HNO_3	Detection Flag
HNO_3	860-920	50% ??	< 1	emissivity	Upper trop
	1320-1330			H_2O, CH_4, N_2O	
N_2O	1250-1315	5% ??	< 1	H_2O	Mid-trop
	2180-2250			H_2O, CO	

5 Validation Needs and Data Sources

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Here we briefly describe several ongoing, recent, and upcoming field campaigns and monitoring programs that can provide data for the validation of current (Section 4) and future (Section 7) CrIS products. We do not attempt to make an exhaustive list of all past and future validation opportunities, but simply demonstrate what required validation data is available. These are organized into campaigns that involve ongoing frequent aircraft flights (Section 5.1), episodic campaigns that are focused on atmospheric chemistry (Section 5.2), long-term surface measurement campaigns (Section 5.3), and campaigns using platforms other than surface sites and aircraft (e.g., balloons, unpiloted aerial vehicles (UAVs), Section 5.4).

While extensive efforts have been made to validate the temperature and H_2O retrieval products from CrIS, very little work has been done to evaluate the trace gas species retrievals. CrIS O_3 retrievals are currently being evaluated using world-wide ozonesonde data from the Southern Hemisphere ADditional OZonesondes (SHADOZ) networks and other sources, and both O_3 and CO products are being evaluated using Measurement of OZone and water vapor on AIrbus in-service airCraft (MOZAIC) and In-service Aircraft for the Global Observing System (IAGOS) aircraft data. Other CrIS trace gas products have not been validated even to this extent. Validating these products with reliable surface, aircraft, balloon, and other data is critical to the scientific and operational use of these products.

While little work has been done to validate CrIS trace gas products to date, a large amount of data from recent and upcoming aircraft, balloon, and surface-based instruments is available for such efforts. For example, the airborne and surface measurement campaigns performed by NOAA ESRL, both by the Chemical Sciences Division (CSD) and the Global Monitoring Division (GMD), are important potential sources for CrIS validation data. Figure 2 shows an example payload for the WP-3 aircraft used by CSD. The payload includes instruments to measure O_3, CO, CO_2, CH_4, NH_3, HNO_3, SO_2, and several other gases that can be detected by CrIS. NOAA ESRL CSD has also provided O_3 and H_2O instruments for a number of NASA and NSF aircraft campaigns. Air samples from aircraft sites in the NOAA ESRL GMD Global Greenhouse Gas Reference Network provide regular measurements of the vertical profiles of CO_2, CH_4, N_2O, and CO over North America and from a single site in the Southern Hemisphere (Raratonga), and continuous O_3 measurements are made on a subset of these flights.

Field campaigns run by other US (e.g., NASA, NCAR, NSF) and international agencies, as well as campaigns organized by university scientists, can also provide a wealth of *in situ* data for the validation of CrIS trace gas retrievals. The CrIS retrieval development and validation community needs to establish stronger ties with the leadership of these US and international field campaigns to ensure, for example, a lineup of data collection with satellite overpass times and rapid access to field data.

Satellite inter-comparisons, such as have been performed for CO and O_3 data from IASI, TES, AIRS, MOPITT, and MLS, can also be useful in identifying problems in new retrieval products. Such inter-comparisons should be extended to include the CrIS trace gas data, but they are not a replacement for rigorous validation efforts with *in situ* measurements and surface remote sensing observations.

In addition, it is recommended that information regarding CrIS be added to the NOAA NESDIS Center for Satellite Applications and Research (STAR) VALAR (VALidation ARchive). VALAR matches validation data from a variety of

sources (sondes, aircraft, etc.) with the corresponding CrIS granule "stamps" that contain the information needed to perform retrieval validation and evaluate updates to retrieval algorithms. Model fields (e.g., from numerical weather prediction models) corresponding to the time and location of the validation data and CrIS retrievals can also be included in VALAR. Once data is placed within VALAR, it can be used to evaluate future improvements to retrieval algorithms.

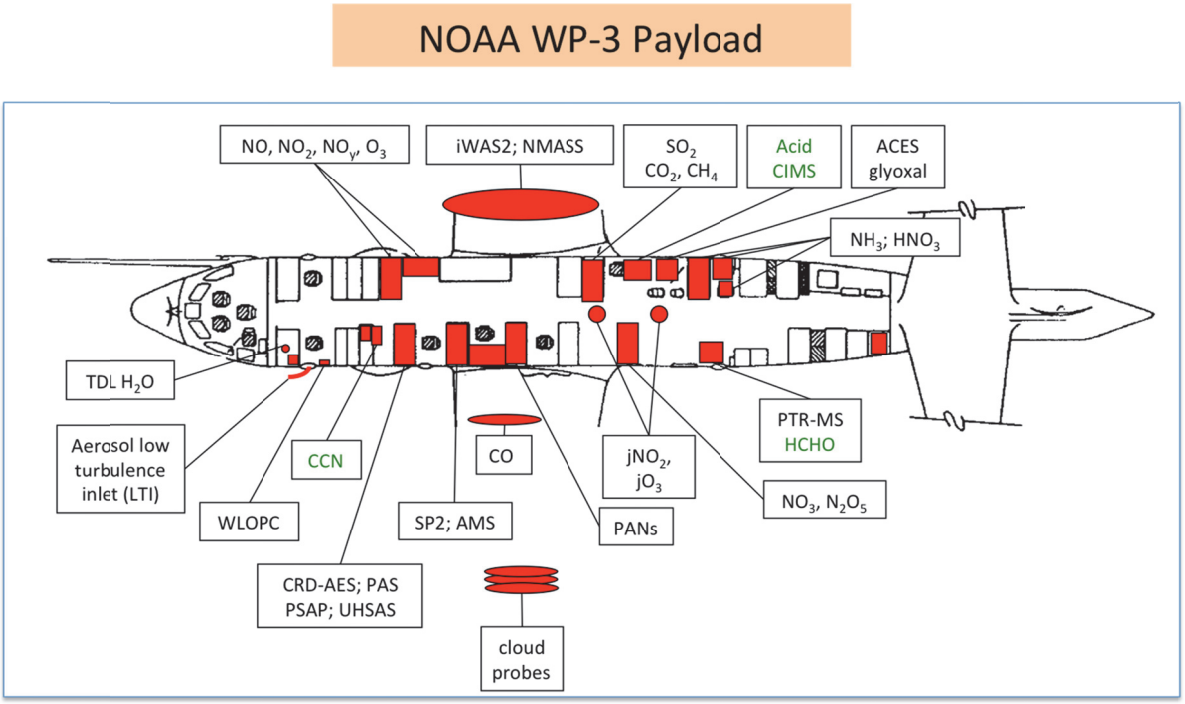

Figure 2. NOAA ESRL CSD WP-3 aircraft with a representative payload.

5.1 Ongoing Measurement Programs

Ongoing campaigns and monitoring programs that have frequent flights, such as those listed below, are critical for providing long-term data on the seasonal and inter-annual changes in trace gas mixing ratios. These flights thus provide a wealth of data for the validation of CrIS retrievals of CO, O_3, CO_2, N_2O, and CH_4, and the CrIS retrieval development and user community should work closely with these teams on validation activities.

The GMD Global Greenhouse Gas Reference Network's aircraft program has been dedicated to collecting air samples in vertical profiles over North America. Most of these flights collect 12 flask samples at different altitudes up to approximately 8 km. These samples are stored in glass flasks for later analysis of CO_2, CO, N_2O, and CH_4, among other gases. These flights are essential to the validation of CrIS retrievals of these gases, and additional flights should be encouraged.

GMD has also been collaborating with the US Coast Guard on a special project in Alaska where a Coast Guard Hercules C-130 aircraft conducts biweekly missions as part of their Arctic Domain Awareness mission, usually flying from Air Station Kodiak up to Barrow and back. The aircraft group at GMD has installed flask packages similar to those described above, a continuous CO2/CH4/H2O analyzer (Picarro), and a continuous O3 monitor (2B Systems) on board this aircraft.

In addition, *GMD* is leading a compilation of aircraft observations of greenhouse gases as part of the CarbonTracker effort. The data will be packaged in a convenient format with point-of-contact information and metadata for individual datasets. An initial data product should be available in 2015.

The Alpha Jet Atmospheric eXperiment (AJAX) Project at NASA Ames makes frequent measurements of the profiles of O3, CH4, and CO2 over California and Nevada up to altitudes >10km in support of NASA's Orbiting Carbon Observatory (OCO-2).

Prof. Takakiyo Nakazawa's group at Tohoku University, in collaboration with the National Institute of Environmental Studies, has measured CO2, CH4, N2O, SF6, CO, and H2 at eight vertical levels using an aircraft in Surgut, Russia since July 1993.

Several research efforts use observing systems aboard passenger aircraft to make frequent observations of atmospheric trace gases covering the major air traffic areas of the globe.

MOZAIC[5] made airborne in-situ measurements for O_3 and CO from August 1994 – November 2014 during round-trip international flights (ascent, descent and cruise phases) from Europe to America, Africa, Middle East, and Asia.

IAGOS[6] is the currently operating follow-on to MOZAIC. This campaign includes observations of O_3 and CO made by five commercial aircraft, with plans to add CH_4 observations and additional aircraft. Aerosol and cloud-particle measurements are also available from IAGOS and may provide information needed to investigate under what conditions aerosols and clouds may interfere with CrIS retrievals.

CARIBIC [7] (Civil Aircraft for the Regular Investigation of the atmosphere Based on an Instrument Container) has been measuring many trace gases, including CO, O_3, CO_2, N_2O, CH_4, CH_3OH, SO_2, C_2H_2, C_2H_4, C_2H_6, and aromatic species aboard an Airbus A340-600 from Lufthansa since 2004.

CONTRAIL [8] (Comprehensive Observation Network for TRace gases by AIrLiner) is a commercial aircraft trace gas sampling program jointly conducted by Japan's NIES (National Institute for Environmental Studies), the MRI (Meteorological Research Institute), JAL (Japan Airlines), JAMCO (JAMCO Corporation), and JAL-F (JAL Foundation). CONTRAIL data includes continuous observations of CO_2 along with whole-air samples analyzed for CO_2, CH_4, CO, and N_2O. Continuous CH_4 measurements are planned for future flights.

[5] http://www.iagos.fr/web/
[6] http://www.iagos.org/IAGOS
[7] http://www.caribic-atmospheric.com
[8] http://www.cger.nies.go.jp/contrail/contrail.html

5.2 Episodic Atmospheric Chemistry Aircraft Campaigns

There were several NOAA, NASA, NSF, and NCAR aircraft campaigns in 2013 and 2014 that measured profiles of some or all of the current and potential future CrIS trace gas retrievals products and thus should be analyzed for validation of the CrIS trace gas retrievals. These campaigns include:

The NOAA CSD SENEX[9] *campaign*, which used the NOAA WP-3 aircraft (see Figure 2, maximum altitude ~6 km) to measure many trace gases in the Southeast US during the summer of 2013. Additional measurements during this time were made from the NSF/NCAR C-130 aircraft as part of the Southeast Atmosphere Study [10], and corresponding surface observations of many trace gases were also made during this period as part of the Southern Oxidant and Aerosol Study (SOAS).

The NASA DISCOVER-AQ[11] *campaign*, (Deriving Information on Surface conditions from Column and Vertically Resolved Observations Relevant to Air Quality) which was a multi-aircraft campaign that had deployments in California (January 2013), Texas (September 2013), and Colorado (summer 2014). These campaigns included *in situ* observations of CO, CO_2, O_3, CH_4, and CH_3OH aboard the NASA P3-B aircraft, along with coordinated surface and aircraft remote sensing observations and ozonesonde launches.

The NASA SEAC[4]*RS*[12] *campaign* (Studies of Emissions and Atmospheric Composition, Clouds and Climate Coupling by Regional Surveys), which was a multi-aircraft campaign during the summer of 2013 that targeted two major regional sources of summertime emissions: intense smoke from forest fires in the US West and natural emissions of isoprene from forests in the Southeast. The NASA DC-8 carried instruments to measure several trace gases, including CO, O_3, CO_2, CH_4, C_2H_6, C_2H_4, C_2H_2, SO_2, and CH_3OH, and the NASA ER-2 made *in situ* measurements of CO, O_3, CO_2, and CH_4. There was also an associated ozonesonde campaign (SEACIONS), and frost point water vapor sondes were launched from Houston during the aircraft campaign.

The NCAR FRAPPE[13] *campaign* (Front Range Air Pollution and Photochemistry Experiment), was in the summer of 2014 concurrent with the NASA DISCOVER-AQ Colorado deployment. In this campaign, the NSF/NCAR C-130 aircraft made *in situ* measurements of CO, O_3, CO_2, CH_4, NH_3, SO_2, HNO_3, HCN, CH_3OH, C_2H_6, C_2H_4, and C_2H_2. The campaign also included ground-based *in situ* and remote sensing measurements made at the Boulder Atmospheric Observatory (BAO) tower, including the UW Atmospheric Emitted Radiance Interferometer (AERI) and radiosonde launches from BAO.

The NASA ESPO (Earth Science Program Office) ATTREX [14] *campaign* (Airborne Tropical TRopopause EXperiment, a NASA Earth Venture mission), which took place over the past 3 years, most recently during winter 2014 based in Guam. This mission used a high altitude unmanned aircraft system (the NASA Global Hawk) to make *in situ* measurements of several trace species in the tropical tropopause, including CO, O_3, CO_2, CH_4, and N_2O.

In addition, there are several upcoming field campaigns in their planning stages that could be used for validation of the CrIS trace gas retrievals, and thus the CrIS retrieval development and atmospheric chemistry user community should closely coordinate with these campaigns:

NOAA ESRL CSD SONGNEX[15] (Shale Oil and Natural Gas NEXus: Studying the Atmospheric

[9] http://www.esrl.noaa.gov/csd/projects/senex/
[10] http://www.eol.ucar.edu/field_projects/sas
[11] http://discover-aq.larc.nasa.gov
[12] http://www.nasa.gov/mission_pages/seac4rs
[13] http://catalog.eol.ucar.edu/frappe
[14] https://espo.nasa.gov/missions/attrex/
[15] http://www.esrl.noaa.gov/csd/projects/songnex/

Effects of Changing Energy Use in the US at the Nexus of Air Quality and Climate Change, March – May 2015), which will use the NOAA WP-3 aircraft based out of Colorado and Texas to investigate the air quality and climate impacts of oil and gas development.

NOAA ESRL CSD FIREX[16] (Fire Influence on Regional and Global Environments Experiment) campaign, which will study the air quality and climate impacts of wildfires and other biomass burning in the US using the NOAA WP-3.

NASA ATom (Atmospheric Tomography), which will use the NASA DC-8 in several campaigns between 2016-2020 to measure trace gases and aerosols in multiple sequential vertical profiles (from the boundary layer to 12 km). From the Armstrong Flight Research Center in Palmdale, California, the aircraft will fly north to the western Arctic, south to the South Pacific, east to the Atlantic, north to Greenland, and return to California across central North America.

NCAR/NSF WINTER[17] *campaign* (Wintertime INvestigation of Transport, Emissions, and Reactivity, January - March 2015), which will use the NSF/NCAR C-130 aircraft and several instruments from NOAA ESRL CSD to make measurements of CO, O_3, CO_2, CH_4, HNO_3, NH_3, and several other gases over the Mid-Atlantic region.

NOAA ESRL CalWater2[18] (January-March 2015), which will use the NOAA G-IV and include the NOAA CSD O_3 instrument as well as water vapor measurements.

CAST (Coordinated Airborne Studies in the Tropics) ATTREX flights (March 2015), which will fly the NASA Global Hawk out of Southern California (NASA Armstrong). These flights will include the NOAA CSD O_3 and H_2O instruments and the GreenHouse Observations of the Stratosphere and Troposphere (GHOST) instrument, which will measure greenhouse gas columns. CAST is funded by the Natural Environment Research Council (NERC) in the United Kingdom.

The planned *NASA Coastal Northwest Pacific Field Study* in 2016, which will include a suite of surface and airborne instruments to validate satellite observations and to examine transboundary transport and modification of gaseous and aerosol pollutants. This campaign will focus on a region of strong gradients driven by large megacity population centers, rural/agricultural areas, and coastal zones.

[16] http://www.esrl.noaa.gov/csd/projects/firex/
[17] http://www.esrl.noaa.gov/csd/groups/csd7/measurements/2015winter/
[18] http://www.esrl.noaa.gov/psd/calwater/

5.3 Surface Measurement Campaigns

Several long-term surface measurement networks make routine measurements of relevant trace gases. These networks include the NOAA ESRL GMD Cooperative Air Sampling Network[19] (which measures CO_2, CH_4, CO, N_2O, and other trace gases) and the NASA Advanced Global Atmospheric Gases Experiment (AGAGE) network (which measures CO, CH_4, N_2O, C_2H_2, C_2H_4, and C_2H_6). Other long-term surface datasets are also available. For example, Prof. Dylan Millet of the University of Minnesota also makes regular tall tower measurements of several trace gas species, including N_2O, acetone, CH_3OH, and CO in the US Upper Midwest [*Griffis et al.,* 2013; *Hu et al.,* 2011, 2013; *Kim et al.,* 2013]. This surface data can also be useful for evaluation of satellite data, either directly or using chemical transport models as a transfer standard. However, direct comparison of surface measurements with TIR retrievals can be complicated because many TIR averaging kernels have maximum sensitivity in the mid-troposphere and low sensitivity to the planetary boundary layer. Careful modeling studies are therefore needed to investigate the consistency of surface and TIR datasets.

In addition to the long-term surface *in situ* measurement campaigns, there are two short-term surface measurement campaigns planned for the near future that could provide useful validation data:

Between April 6 and May 13, 2015, a research *team led by Prof. Robert Yokelson at the University of Montana* will be conducting a ground-based field campaign in Nepal, measuring surface concentrations and emission ratios of combustion sources for many chemical species including, but not limited to, aerosols, H_2O, CO_2, CO, CH_4, NH_3, C_2H_2, C_2H_4, C_3H_6, O_3, and SO_2.

Prof. Emily Fischer and Prof. Delphine Farmer at Colorado State University have two measurements campaigns planned for the BAO tower. These are planned for mid-March – early-May 2015 (firm) and July – August 2015 (tentative). These will provide boundary layer profiles (surface to 300 m) of CH_4, CO, CO_2 and H_2O.

Furthermore, surface remote sensing instruments can also be used for satellite validation. For example, the Total Carbon Column Observing Network[20] (TCCON) obtains total column amounts of CO_2 and other greenhouse gases and has been used as a validation method for other satellite instruments, while sites in the Network for the Detection of Atmospheric Composition Change (NDACC)[21] include FTIR retrievals of many trace gases such as CH_4, N_2O, H_2O, and O_3, along with LiDAR O_3 profiles and ozonesonde launches at several sites. The planned Global Climate Observing System (GCOS) Reference Upper-Air Network (GRUAN) sites[22] will also provide quality-controlled profiles of temperature, winds, water vapor, and ozone. In addition, the University of Wisconsin-Madison SSEC, in collaboration with NESDIS, has capabilities for mobile deployment of various ground-based remote sensing instruments including the SSEC High Spectral Resolution LiDAR (HSRL) and the AERI, which were recently deployed at the NOAA Boulder Atmospheric Observatory during FRAPPE.

[19] http://www.esrl.noaa.gov/gmd/ccgg/flask.php

[20] http://www.tccon.caltech.edu

[21] http://www.ndsc.ncep.noaa.gov

[22] http://www.wmo.int/pages/prog/gcos/index.php?name=GRUAN

5.4 Other Platforms

In addition to the surface and aircraft measurements mentioned above, weather balloon networks around the globe are used to carry a variety of trace gas instruments that can be useful for validation of CrIS trace gas retrievals. For example, ozonesonde and ground-based remote sensing data collected under the Network for Detection of Atmospheric Composition Change (NDACC)[23] have long served for evaluation satellite measurements of O_3. Regional augmentation is provided by the NDACC cooperating network SHADOZ campaign run by Dr. Anne Thompson of NASA GSFC (Goddard Space Flight Center), which has long-term records of ozonesonde data from multiple locations in the tropics and southern hemisphere [*Thompson et al.,* 2003a,b, 2007].

The NOAA ESRLGMD AirCore sampling system for CO, CO_2, CH_4, and other trace gases [*Karion et al.,* 2010] can be used on a variety of platforms, including balloons, UAVs and aircraft. It uses a long stainless steel tube, open at one end and closed at the other. The AirCore evacuates while ascending to a high altitude and collects a sample of the ambient air as it descends. It is sealed upon recovery and measured with a continuous analyzer for trace gas mole fraction. Presently about 20 vertical profiles of trace gases are collected globally each week by NOAA ESRL.

Remote sounders for balloon platforms can also be used for validation; one example is the JPL Mark IV Balloon Interferometer [24] of Dr. Geoffrey Toon (flown most recently in Sept. 2014). Sophisticated *in situ* instruments, such as the NOAA ESRL GMD Unmanned Aircraft Systems (UAS) Chromatograph for Atmospheric Trace Species (UCATS), are also ready to fly. In addition, balloons can be launched from ships to assist in the validation of H_2O and O_3 over the ocean, such as in the NOAA AEROSE (AERosols and Ocean Science Expeditions) campaign, which uses the blue-water NOAA ship *Ronald H. Brown* to acquire simultaneous *in situ* and remotely sensed marine data during intensive observing periods in the tropical Atlantic. This campaign includes the launch of radiosondes and ozonesondes. NOAA ESRL CSD and GMD are also currently developing small, inexpensive packages to measure ozone and aerosols from balloons or UAVs. These packages could be used for validation in the future.

[23] http://www.ndsc.ncep.noaa.gov/

[24] https://espo.nasa.gov/missions/instrument/MkIV

6 Product Changes and Refinements

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6.1 Current Product Format and Distribution

The NUCAPS Environmental Data Record (EDR) product can be ordered from CLASS under the data family Suomi-NPP Data Exploitation Granule Data (NDE_L2) [25]. The CLASS (Comprehensive Large Array-data Stewardship System) product distribution has a latency period of about 3 hours. The NUCAPS EDR product consists of retrieved estimates of hydrological variables including temperature, water vapor, cloud fraction, and cloud top pressure, along with the following 100-level trace gas profiles calculated on each CrIS field-of-regard (i.e., the 3x3 array of individual 14 km circle fields-of-view):

- O_3 layer column density
- O_3 mixing ratio
- First Guess O_3 layer column density
- First Guess O_3 mixing ratio
- CH_4 layer column density
- CH_4 mixing ratio
- CO_2 mixing ratio
- HNO_3 layer column density
- HNO_3 mixing ratio
- CO layer column density
- CO mixing ratio
- N_2O layer column density
- N_2O mixing ratio
- SO_2 layer column density
- SO_2 mixing ratio

The NUCAPS EDR products are distributed in netCDF-4 file format with metadata attributes included. Each file contains one 32-second granule of CrIS data.

To obtain the near real time NUCAPS data, a user needs to fill out the Data Access Request Form located at the OSPO web site[26] and submit it to the Sounding Product Area Lead (awdhesh.sharma@noaa.gov) with a copy to nesdis.data.access@noaa.gov.

Real-time NUCAPS products can also be generated locally on user systems by running the NUCAPS retrieval software prepared by the University of Wisconsin (UW)-Madison as part of the stand-alone, open-source CSPP. From February 2015 onwards, CSPP [27] (a NOAA funded UW-Madison initiative) will distribute the NUCAPS algorithm as a stand-alone software package to any registered user, from scientific to direct-broadcast. In addition, any changes to the NUCAPS science code can be distributed as a CSPP version to the scientific community for testing and evaluation. This has the potential to speed up and streamline algorithm development, as CSPP NUCAPS can be used to explore algorithm changes and product enhancements without incurring too much cost or degrading the operational data stream with invalidated/interim science products. The CSPP distribution of NUCAPS has the added advantage that users can reprocess historic data with the latest operational algorithm updates. This feature is especially important for climate studies.

[25] http://www.nsof.class.noaa.gov/saa/products/search?sub_id=0&datatype_family=NDE_L2&submit.x=25&submit.y=11

[26] www.ospo.noaa.gov/Organization/About/access.html

[27] http://cimss.ssec.wisc.edu/cspp/

6.2 Recommended Refinements

One of the key limitations of the current NUCAPS EDR files is that there is insufficient data provided to construct an observation operator for each trace gas retrieval, as is needed for most atmospheric chemistry applications [e.g., *Jones et al*., 2003; *Migliorini et al.,* 2008]. The observation operator allows an atmospheric profile of a gas, either from *in situ* measurements [e.g., *Worden, H. M. et al*., 2007] or a model, to be converted into the corresponding profile that would have been retrieved by the satellite, accounting for the vertical smoothing errors and *a priori* information of the retrieval process. For optimal estimation retrievals, this observation operator is a function of the averaging kernel and *a priori* profile [e.g., *Rodgers and Connor*, 2003]. The main reason this data is not already provided in the NUCAPS EDR is that storing the 100 level *a priori* profiles and 100x100 averaging kernel (AK) arrays for each trace gas retrieval would make the file size prohibitively large for the CLASS archive.

However, there are now several methods for reducing the size of the data that are needed to rebuild the observation operator. For example, the AK array could be reconstructed from singular vectors following a singular value decomposition (SVD) processing step. This would result in array sizes of 100x2N + N, where N is the number of singular values retained, with left singular vector (**U** = Nx100), right singular vector (**V** = Nx100) and the singular values (N) to form a diagonal matrix **Λ (**NxN**)**. The AK (**A**) is then reconstructed with:

$$\mathbf{A} = \mathbf{U}\,\mathbf{\Lambda}\,\mathbf{V}^{T}$$

For typical O_3 AKs from thermal IR sensors, N~8 in order to maintain errors less than ~2% in the reconstructed AK, which would reduce the size from 10000 to ~1608. For typical TIR CO AKs, N~4 [*Worden, H.M. et al.,* 2013b], corresponding to a 92% reduction in the AK size.

Although most analytical data users would require the observation operator for each trace gas retrieval (such as for data assimilation applications), it would also be useful to provide average *a priori* profiles and typical AKs by region and observation type (e.g., latitude range, land/ocean, day/night). These could be available on a website and would allow users to determine if the retrievals are suitable for their analyses. They would also provide guidance for users that are reconstructing the AKs from SVD information.

In addition, most atmospheric chemistry users of CrIS data will not need the full vertical resolution of 100 vertical levels, nor will they require both the mixing ratio profile and the profile of the layer column density (as the second is mainly useful for radiative transfer modeling). Thus we recommend that rather than adding observation operators, etc., to the existing EDR files, NESDIS STAR should provide reduced files, modeled on the TES "lite" products available at the JPL TES web site[28], that provide the retrievals for individual trace gases and their observation operators (i,e., averaging kernels compressed as described above and *a priori* profiles) at a reduced vertical resolution sufficient to capture the vertical variations in each species. These lite files would contain all the data for a given species for a to-be-determined chunk of time (e.g., one day) for easier manipulation and would be *in addition to* the granule files provided at the full vertical resolution of the CrIS forward radiative transfer model through CLASS (as described above). The TES "lite" files are in NetCDF format and contain all the observations for a single trace gas in a month. A similar IASI "lite" product[29] provides daily text files (instead of monthly, reflecting the larger volume of data) containing IASI CO data on a reduced vertical grid. This product includes retrieved total column density, the *a priori* profile on 19 layers, the averaging kernel

[28] http://tes.jpl.nasa.gov/data/

[29] Available at http://www.pole-ether.fr/etherTypo/index.php?id=1585&L=1

diagonal vector on 19 layers, and the total degrees of freedom of signal.

For TES, known bias corrections to the retrieved profiles are applied before preparing the "lite" products. Any bias corrections applied should be clearly documented in either the lite files themselves (e.g., by providing an uncorrected profile along with the corrected profile) or in the accompanying users guide. To facilitate the use of the data, the CLASS archive should be updated to support easy multi-file download of these lite products, rather than the current limits of 100-500 granule files in your "shopping cart", through tools such as the "wget" utility used by NASA. Example routines for reading the data files in FORTRAN, IDL, and other commonly used analysis tools should also be provided. Finally, a CrIS trace gas users' guide should be compiled with recommended quality flags and other techniques to facilitate the use of the data and should be provided along with the lite product files.

7 Potential New Products

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7.1 Products Needed to Continue the Records of Other TIR Sounders

7.1.1 Methanol

Methanol is the most abundant non-methane organic gas in the atmosphere and an important source of tropospheric formaldehyde and carbon monoxide. Space-based TIR methanol measurements provide powerful information for diagnosing the sources of methanol to the atmosphere as well as the subsequent impacts on atmospheric chemistry [*Stavrakou et al.,* 2011; *Wells et al.*, 2012, 2014]. Since terrestrial plants provide the dominant net source of atmospheric methanol, such measurements can also inform our understanding of ecosystem processes and provide a biogenic tracer for distinguishing sources of other atmospheric species.

7.1.2 Instantaneous Radiative Kernels (IRKs)

Using CrIS radiances, Jacobians and ozone profiles with hemispherical integration, it is possible to compute the TOA (Top-Of-Atmosphere) flux from the infrared ozone band (in W/m^2) along with instantaneous radiative kernels (IRKs) (in $W/m^2/ppb$). The IRK provides unique information for questions of chemistry-climate coupling, since this is a direct measure of the sensitivity of the TOA flux to the ozone distribution. The IRK explicitly accounts for more dominant radiative processes such as clouds and water vapor due to the spectrally resolved absorption features. These ozone band flux and IRK products can be compared to climate model predictions of the same quantities and can allow evaluation of model processes that affect ozone radiative forcing [*Worden, H. M. et al.,* 2008, 2011; *Bowman and Henze*, 2012; *Bowman et al.,* 2013]. These products from TES have been applied to climate model evaluation for the NASA GFSC GISS Atmospheric Chemistry and Climate Model Intercomparison Project (ACCMIP) [*Lamarque et al.,* 2013; *Bowman et al.*, 2013] and incorporated into the findings of the IPCC (Intergovernmental Panel on Climate Change) AR5 (Fifth Assessment Report) [*Myhre et al.,* 2014].

7.2 Possible New Products from CrIS

7.2.1 Dust

Dust particles affect atmospheric radiative transfer in both the short-wave and long-wave spectrum and hence are important for the prediction of climate and weather. However, characterization of dust from space can be complicated by the factors such as dust particle size and morphology and the vertical distribution of dust, as well as surface characteristics (especially bright desert). Past remote sensing of dust has used the visible spectrum (primarily over the ocean and dark/vegetated surfaces, as in the MODIS Dark Target algorithm [*Levy et al.,* 2007]), the UV-blue spectrum (with strengths over visibly bright or arid/semi-arid surfaces, as in the MODIS Deep Blue Algorithm [*Hsu et al.,* 2006]), the OMI UV algorithm [*Torres et al.,* 2007], and the infrared spectrum [*Ackerman,* 1997]. In addition, *Pierangelo et al.* [2004, 2005] have demonstrated the use of thermal infrared

spectra to retrieve dust optical depth, size, and altitude from AIRS over the ocean. Each technique has its own strengths and weakness, but none of these techniques can retrieve the dust optical depth, absorption, particle size, and centroid height at the same time. By combining hyperspectral measurements from the Ozone Mapping Profiler Suite (OMPS, UV-visible) and CrIS (short-wave and thermal infrared), there are opportunities to have a consistent retrieval algorithm that can be applied globally to better characterize dust properties, including their optical depth, single scatting albedo, and centroid height over both visibly dark and bright surfaces.

7.2.2 Ethane

Ethane is ubiquitously present in the atmosphere. It is the second largest component of natural gas after methane, and the bulk of its emissions are associated with natural gas production, distribution, and processing [*Xiao et al.,* 2008]. As such, observations of atmospheric ethane can yield critical insights into the global methane budget and the changing role of fossil fuels as a methane source [e.g., *Simpson et al.,* 2012; *Aydin et al.,* 2011]. Furthermore, sustained ethane measurements can help constrain the seasonal and spatial distribution of atmospheric OH, the main sink for most atmospheric pollutants and greenhouse gases [e.g., *Goldstein et al.,* 1995].

7.2.3 Acetylene

Acetylene (C_2H_2), the lightest non-methane hydrocarbon, has similar sources as CO; both are emitted from incomplete combustion of fossil fuel, biofuel, and biomass. C_2H_2 and CO are also both removed by reaction with OH radicals. C_2H_2 is shorter-lived than CO (with a mean global lifetime of 2 weeks versus 2 months), but persistently strong C_2H_2-CO correlations are seen in atmospheric observations extending to the remote troposphere. Such C_2H_2/CO ratios can be used as a diagnostic of air mass "age" following the last encounter of an air mass with a combustion source region. C_2H_2/CO ratios can also be used to constrain OH concentrations [*Xiao et al.,* 2007], and as C_2H_2 does not have secondary chemical sources in the atmosphere, C_2H_2 could be used to help quantify the secondary source of CO from, for example, isoprene oxidation.

7.2.4 HCN

Hydrogen cyanide (HCN) is an important tracer for biomass burning emissions. *Duflot et al.* [2013] showed that IASI can determine the ratio of HCN to CO in a biomass burning plume, and the lower noise of CrIS in the long-wave band should allow the detection of even lower concentrations of HCN. Co-located CrIS retrieval of HCN with retrievals of CO, CH_4, and other gases would help to constrain the contribution of biomass burning to the budgets of these gases.

7.2.5 Ethylene

Ethylene (C_2H_4) is a highly reactive hydrocarbon that is generally concentrated in the lower troposphere [*Rinsland et al.,* 2005] and is emitted directly by biomass burning [*Akagi et al.,* 2011]. Other sources of C_2H_4 include biogenic emissions from plants and the ocean, the anthropogenic burning of fossil fuels and biomass, and petrochemical facilities [e.g., *Goldstein et al.*, 1996; *Broadgate et al.,* 1997; *Folberth et al.,* 2006]. Urban centers often have high ethylene concentrations [e.g., *Altuzar et al.,* 2001] due to production by cars and trucks.

C_2H_4 has a short lifetime due to rapid reaction with OH, and its high reactivity and oxidation products make it a key precursor of O_3 in urban smog [e.g., *Jiang and Fast*, 2004] and in biomass burning plumes [*Alvarado and Prinn,* 2009].

There have been several previous studies that have detected a C_2H_4 signal in TIR radiance spectra measured by aircraft and satellite instruments. *Worden et al.* [1997] detected enhanced mixing ratios of C_2H_4 from forest fires near San Luis Obispo, California, on 15 August 1994 using the Airborne Emission Spectrometer (AES), the airborne prototype for TES. Enhanced mixing ratios of C_2H_4 from biomass burning have also been detected by the limb-viewing Atmospheric Chemistry Experiment Fourier Transform Spectrometer (ACE-FTS) [*Coheur et al*., 2007] and the nadir-viewing IASI [*Coheur et al*., 2009; *Clarisse et al.,* 2011]. *Alvarado et al.* [2011] presented the first detection of C_2H_4 from TES, in a fresh Canadian biomass burning plume observed in the summer of 2008 as part of the Arctic Research of the Composition of the Troposphere from Aircraft and Satellites (ARCTAS-B) campaign. TES also detected the residual feature of C_2H_4 during the biomass burning season in tropical South America.

7.2.6 Acetic and Formic acids

Formic and acetic acids are the dominant carboxylic acids in the atmosphere. They exert an important influence on atmospheric aqueous chemistry through their effect on the pH of precipitation, aqueous OH radical concentrations, and possibly secondary organic aerosol (SOA) production [*Keene et al.,* 1983; *Keene and Galloway,* 1984; *Jacob,* 1986; *Andreae et al.,* 1998; *Millet et al.,* 2015]. Recent work, including analyses of TES satellite retrievals of formic acid, has shown that the atmospheric abundance of both compounds is substantially larger than can be explained based on current understanding of their budgets [*Cady-Pereira et al*., 2014; *Le Breton et al*., 2012; *Paulot et al.,* 2011*; Stavrakou et al*., 2012]. In turn, this points to a key gap in present understanding of the atmospheric reactive carbon budget. Atmospheric measurements for both species are extremely limited, and space-based TIR measurements are needed to close the budgets of atmospheric carboxylic acids, quantify their impacts in the atmosphere, and improve current mechanisms of atmospheric hydrocarbon oxidation [*Stavrakou et al*., 2012]. The exceptionally low noise of CrIS could allow the retrieval of atmospheric acetic acid. While the CrIS instrument aboard Suomi-NPP does not include the channels needed to retrieve HCOOH, closing this spectral gap for JPSS-2 and beyond would allow the continuation of retrievals for this important trace gas (see Section 7.3 below).

7.2.7 Benzene

Aromatic volatile organic compounds (VOCs) such as benzene (C_6H_6), toluene (C_7H_8), xylenes (C_8H_{10}; including o-, m-, p- isomers), and ethylbenzene (also C_8H_{10}) are ubiquitous in the atmosphere and are important anthropogenic precursors of SOAs [*Johnson et al.*, 2005; *Martín-Reviejo and Wirtz*, 2005; *Ng et al.,* 2007; *Henze et al.,* 2008], PAN [*Liu et al.,* 2010], and, to a lesser degree, ground-level ozone [*Ahmadov et al.,* 2014; *Jaars et al.,* 2014; *Xue et al.,* 2014]. These aromatic VOCs (so-called BTEX compounds) are categorized as hazardous air pollutants (HAPs) under the US Clean Air Act Amendments of 1990, as they are known or suspected to cause serious health effects. For instance, benzene is classified as a Group 1 carcinogen by the International Agency for Research on Cancer [*Baan et al.*, 2009]. Despite their importance, emissions of aromatic compounds remain poorly quantified [e.g., *Hu et al.,* 2014; *Liu et al*., 2012]. Globally continuous measurements of benzene and other aromatic species from CrIS would provide unique and powerful information for quantifying emissions of aromatics and their environmental and health impacts.

7.3 Additional Products Possible if JPSS-2 Spectral Gap Were Closed

The current spectral gap between the long-wave and mid-wave bands in the Suomi-NPP CrIS instrument prevents the retrieval of two important trace gases, HCOOH and PAN, that are currently retrieved by TIR sounders [e.g., *Payne et al.,* 2014; *Cady-Pereira et al.,* 2014]. As noted in Section 7.2.6 above, formic acid is ubiquitous in the atmosphere. Our understanding of its chemical formation in the atmosphere is poor, partially due to the limited atmospheric observations available. Satellite observations of formic acid with extensive spatial coverage, such as would be possible with the CrIS instrument if the spectral gaps were closed, are thus needed to understand the chemical formation of this gas in order to improve our understanding of atmospheric oxidation of organic compounds in general.

PAN, formed when non-methane volatile organic compounds (NMVOCs) are oxidized in the atmosphere in the presence of NO_x, is a major reservoir of nitrogen oxide radicals (NO_x) in the troposphere. It affects the global distribution of O_3 through the transport and release of NO_x to the remote troposphere. Global satellite observations of PAN have the potential to dramatically improve our understanding of O_3 production and transport. PAN has previously been retrieved in the upper troposphere from the Envisat Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) instrument and the Canadian ACE-FTS [*Moore and Remedios*, 2010; *Tereszchuk et al.,* 2013]. PAN has also been observed in fire plumes by the TES instrument on the Aura satellite [*Alvarado et al.,* 2011] and by the MetOp-A IASI [*Coheur et al.,* 2009]. *Payne et al.* [2014] represents the first retrievals of PAN in the nadir view on the global scale. As discussed above, this new data is being used to address a number of open questions with respect to the sources and global distribution of PAN. A CrIS PAN product would immediately be of benefit because CrIS has better spatial coverage than TES, and the lower noise may also allow a lower detection limit for this species. TES is able to detect only elevated (< 200 pptv) PAN mixing ratios. Based on model calculations [e.g. *Fischer et al*., 2014], much of the troposphere has PAN mixing ratios below 200 pptv.

7.4 Validation of New Products

All the products listed in Sections 7.1, 7.2, and 7.3 are currently measured in-situ, many on aircraft and balloon platforms.

See the Section 5 on recent and upcoming validation campaigns for more details.

8 References

Ackerman, S. A. (1997), Remote sensing aerosols using satellite infrared observations, J. Geophys. Res., 102, 17,069–017,079.

Aghedo, A. M., K. W. Bowman, D. T. Shindell, and G. Faluvegi (2011), The impact of orbital sampling, monthly averaging and vertical resolution on climate chemistry model evaluation with satellite observations, Atmos. Chem. Phys., 11(13), 6493–6514, doi:10.5194/acp-11-6493-2011.

Ahmadov, R., S. McKeen, M. Trainer, R. Banta, A. Brewer, S. Brown, P. M. Edwards, J. A. de Gouw, G. J. Frost, J. Gilman, D. Helmig, B. Johnson, A. Karion, A. Koss, A. Langford, B. Lerner, J. Olson, S. Oltmans, J. Peischl, G. Pétron, Y. Pichugina, J. M. Roberts, T. Ryerson, R. Schnell, C. Senff, C. Sweeney, C. Thompson, P. R. Veres, C. Warneke, R. Wild, E. J. Williams, B. Yuan, and R. Zamora (2014), Understanding high wintertime ozone pollution events in an oil and natural gas producing region of the western US, Atmos. Chem. Phys. Discuss., 14(14), 20295–20343, doi:10.5194/acpd-14-20295-2014.

Akagi, S. K., R. J. Yokelson, C. Wiedinmyer, M. J. Alvarado, J. S. Reid, T. Karl, J. D. Crounse, and P. O. Wennberg (2011), Emission factors for open and domestic biomass burning for use in atmospheric models, Atmos. Chem. Phys., 11, 4039-4072, doi:10.5194/acp-11-4039-2011.

Altuzar, V., M. Pacheco, S. A. Tomas, J. L. Arriaga, O. Zelaya-Angel, and F. Sanchez-Sinencio (2001), Analysis of Ethylene Concentration in the Mexico City Atmosphere by Photoacoustic Spectroscopy, Analytical Sciences, 17, s541-s543.

Alvarado, M. J., and R. G. Prinn (2009), Formation of Ozone and Growth of Aerosols in Young Smoke Plumes from Biomass Burning, Part 1: Lagrangian Parcel Studies, J. Geophys. Res., 114, D09306, doi:10.1029/2008JD011144.

Alvarado, M. J., K. E. Cady-Pereira, Y. Xiao, D. B. Millet, and V. H. Payne (2011), Emission ratios for ammonia and formic acid and observations of peroxy acetyl nitrate (PAN) and ethylene in biomass burning smoke as seen by the Tropospheric Emission Spectrometer (TES), Atmosphere, 2(4), 633–654.

Andreae, M. O., R. W. Talbot, T. W. Andreae, and R. C. Harriss (1988), Formic and acetic acid over the central Amazon region, Brazil: 1. Dry season, J. Geophys. Res., 93, 1616–1624.

Aydin, M., K. R. Verhulst, E. S. Saltzman, M. O. Battle, S. A. Montzka, D. R. Blake, Q. Tang, and M. J. Prather (2011), Recent decreases in fossil-fuel emissions of ethane and methane derived from firn air, Nature, 476, 198–201.

Baan, R., Y. Grosse, K. Straif, B. Secretan, F. El Ghissassi, V. Bouvard, L. Benbrahim-Tallaa, N. Guha, C. Freeman, L. Galichet, and V. Cogliano (2009), A review of human carcinogens—Part F: Chemical agents and related occupations, Lancet Oncol., 10(12), 1143–1144, doi:10.1016/S1470-2045(09)70358-4.

Bowman, K., and D. K. Henze (2012), Attribution of direct ozone radiative forcing to spatially resolved emissions, 39(22), L22, 704, doi:10.1029/2012GL053274.

Bowman, K.W., C. D. Rodgers, S. S. Kulawik, J. Worden, E. Sarkissian, G. Osterman, T. Steck, M. Lou, A. Eldering, M. Shephard, H. Worden, M. Lampel, S. Clough, P. Brown, C. Rinsland, M. Gunson, and R. Beer (2006), Tropospheric emission spectrometer: retrieval method and error analysis, *IEEE Trans. Geosci. Remote Sens.*, 44, 1297-1307, doi: 10.1109/TGRS.2006.871234.

Bowman, K. W., D. B. A. Jones, J. A. Logan, H. Worden, F. Boersma, R. Chang, S. Kulawik, G. Osterman, P. Hamer, and J. Worden (2009), The zonal structure of tropical O3 and CO as observed by the Tropospheric Emission Spectrometer in November 2004 – Part 2: Impact of surface emissions on O3 and its precursors, Atmos. Chem. Phys., 9, 3563–3582, doi:10.5194/acp-9-3563-2009.

Bowman, K. W., R. Baron, J. Al-Saadi, A. Arellano, J. Blaisdell, M. Chahine, C. Clerbaux, P. DeCola, S. Hannon, M. Kopacz, E. Maddy, E.

Olsen, L. Ott, B. Pierce, N. Pougatchev, I. Stajner, A. Tangobrn, J. Xun, and L. Yurganov (2011), NASA Science Community Workshop on Polar Orbiting IR and MW Sounders Breakout Session 2: Atmospheric Composition, available at http://airs.jpl.nasa.gov/events/33

Bowman, K. W., D. T. Shindell, H. M. Worden, J. F. Lamarque, P. J. Young, D. S. Stevenson, Z. Qu, M. de la Torre, D. Bergmann, P. J. Cameron-Smith, W. Collins, R. Doherty, S. B. Dalsøren, G. Faluvegi, G. Folberth, L. W. Horowitz, B. Josse, Y. H. Lee, I. A. MacKenzie, G. Myhre, T. Nagashima, V. Naik, D. A. Plummer, S. T. Rumbold, R. B. Skeie, S. A. Strode, K. Sudo, S. Szopa, A. Voulgarakis, G. Zeng, S. S. Kulawik, A. M. Aghedo, and J. R. Worden (2013), Evaluation of ACCMIP outgoing longwave radiation from tropospheric ozone using TES satellite observations, Atmos. Chem. Phys.13(8), 4057–4072, doi:10.5194/acp-13-4057-2013.

Broadgate, W. J., P. S. Liss, and S. A. Penkett (1997), Seasonal emissions of isoprene and other reactive hydrocarbon gases from the ocean, Geophys. Res. Lett., 24, 2675–2678, doi:10.1029/97GL02736.

Cady-Pereira, K. E., M. W. Shephard, D. B. Millet, M. Luo, K. C. Wells, Y. Xiao, V. H. Payne, and J. Worden (2012), Methanol from TES global observations: retrieval algorithm and seasonal and spatial variability, Atmos. Chem. Phys., 12, 8189–8203.

Cady-Pereira, K. E., S. Chaliyakunnel, M. W. Shephard, D. B. Millet, M. Luo, and K. C. Wells (2014), HCOOH measurements from space: TES retrieval algorithm and observed global distribution, Atmos. Meas. Tech., 7, 2297–2311.

Chaliyakunnel, S., D. B. Millet, K. C. Wells, K. E. Cady-Pereira, and M. W. Shephard (2013), Global formic acid measurements from space: The importance of biomass burning emissions, Abstract A31C-0098 presented at the 2013 Fall Meeting, AGU, San Francisco, Calif., 9-13 Dec.

Clarisse, L., Y. R'Honi, P.-F. Coheur, D. Hurtmans, and C. Clerbaux (2011), Thermal infrared nadir observations of 24 atmospheric gases, Geophys. Res. Lett., 38, L10802, doi:10.1029/2011GL047271.

Coheur, P.-F., H. Herbin, C. Clerbaux, D. Hurtmans, C. Wespes, M. Carleer, S. Turquety, C. P. Rinsland, J. Remedios, D. Hauglustaine, C. D. Boone, and P. F. Bernath (2007), ACE-FTS observation of a young biomass burning plume: first reported measurements of C_2H_4, C_3H_6O, H_2CO and PAN by infrared occultation from space, Atmos. Chem. Phys., 7, 5437-5446, doi:10.5194/acp-7-5437-2007.

Coheur, P.-F., L. Clarisse, S. Turquety, D. Hurtmans, and C. Clerbaux (2009), IASI measurements of reactive trace species in biomass burning plumes, Atmos. Chem. Phys., 9, 5655–5667, doi:10.5194/acp-9-5655-2009.

Crevoisier, C., D. Nobileau, R. Armante, L. Crépeau, T. Machida, Y. Sawa, H. Matsueda, T. Schuck, T., Thonat, J. Pernin, N. A. Scott, and A. Chédin (2013), The 2007–2011 evolution of tropical methane in the mid-troposphere as seen from space by MetOp-A/IASI, Atmos. Chem. Phys., 13, 4279–4289, doi:10.5194/acp-13-4279-2013, 2013.

Deeter, M. N., L. K. Emmons, G. L. Francis, D. P. Edwards, J. C. Gille, J. X. Warner, B. Khattatov, D. Ziskin, J.-F. Lamarque, S.-P. Ho, V. Yudin, J.-L. Attié, D. Packman, J. Chen, D. Mao, and J. R. Drummond (2003), Operational carbon monoxide retrieval algorithm and selected results for the MOPITT instrument, J. Geophys. Res., 108(D14), 4399, doi:10.1029/2002JD003186.

Deeter, M. N., D. P. Edwards, and J. C. Gille (2007), Retrievals of carbon monoxide profiles from MOPITT observations using lognormal a priori statistics, J. Geophys. Res., 112, D11311, doi:10.1029/2006JD007999.

Duflot, V., D. Hurtmans, L. Clarisse, Y. R'honi, C. Vigouroux, M. De Mazière, E. Mahieu, C. Servais, C. Clerbaux, and P.-F. Coheur (2013), Measurements of hydrogen cyanide (HCN) and acetylene (C_2H_2) from the Infrared Atmospheric Sounding Interferometer (IASI), Atmos. Meas. Tech., 6, 917–925, doi:10.5194/amt-6-917-2013.

Emmons, L. K., S. Walters, P. G. Hess, J.-F. Lamarque, G. G. Pfister, D. Fillmore C.

Granier, A. Guenther, D. Kinnison, T. Laepple, J. Orlando, X. Tie, G. Tyndall, C. Wiedinmyer, S. L. Baughcum, and S. Kloster (2010), Description and evaluation of the Model for Ozone and Related chemical Tracers, version 4 (MOZART-4), Geosci. Model Dev., 3, 43-67, doi:10.5194/gmd-3-43-2010.

Fischer, E. V., D. J. Jacob, R. M. Yantosca, M. P. Sulprizio, D. B. Millet, J. Mao, F. Paulot, H. B. Singh, A. Roiger, L. Ries, R. W. Talbot, K. Dzepina, and S. Pandey Deolal (2014), Atmospheric peroxyacetyl nitrate (PAN): a global budget and source attribution, Atmos. Chem. Phys., 14, 2679–2698, doi:10.5194/acp-14-2679-2014.

Flemming, J., V-H. Peuch, R. Engelen, and J. W. Kaiser (2013), A European Global-to-Regional Air Pollution Forecasting System that Combines Modeling with Satellite Observations, EM November 2013, published by the Air & Waste Management Association.

Folberth, G. A., D. A. Hauglustaine, J. Lathière, and F. Brocheton (2006), Interactive chemistry in the Laboratoire de Météorologie Dynamique general circulation model: model description and impact analysis of biogenic hydrocarbons on tropospheric chemistry, Atmos. Chem. Phys., 6, 2273-2319, doi:10.5194/acp-6-2273-2006.

Gambacorta, A. and C. Barnet (2013), Methodology and information content of the NOAA NESDIS operational channel selection for the Cross-Track Infrared Sounder (CrIS), IEEE Trans. Geosci. Remote Sens., 51(6), 3207–3216.

Goldstein, A. H., S. C. Wofsy, and C. M. Spivakovsky (1995), Seasonal variations of nonmethane hydrocarbons in rural New England: Constraints on OH concentrations in northern midlatitudes, J. Geophys. Res., 100(D10), 21023–21033, doi:10.1029/95JD02034.

Goldstein, A. H., S. M. Fan, M. L. Goulden, J. W. Munger, S. C. Wofsy (1996), Emissions of ethene, propene, and *1*-butene by a midlatitude forest, J. Geophys. Res., 101(D4), 9149–9157, doi:10.1029/96JD00334.

Griffis, T. J., X. Lee, J. M. Baker, M. P. Russelle, X. Zhang, R. Venterea, and D. B. Millet (2013), Reconciling the differences between top-down and bottom-up estimates of nitrous oxide emissions for the US Corn Belt, Global Biogeochem. Cy., 27, 1–9, doi:10:1002/gbc.20066.

Heald, C. L., J. L. Collett Jr., T. Lee, K. B. Benedict, F. M. Schwandner, Y. Li, L. Clarisse, D. R. Hurtmans, M. Van Damme, C. Clerbaux, P.-F. Coheur, S. Philip, R. V. Martin, and H. O. T. Pye (2012), Atmospheric ammonia and particulate inorganic nitrogen over the United States, Atmos. Chem. Phys. Discuss., 12, 19455–19498.

Henze, D. K., J. H. Seinfeld, N. L. Ng, J. H. Kroll, T. M. Fu, D. J. Jacob, and C. L. Heald (2008), Global modeling of secondary organic aerosol formation from aromatic hydrocarbons: high- vs. low-yield pathways, Atmos. Chem. Phys., 8(9), 2405–2420, doi:10.5194/acp-8-2405-2008.

Hsu, N. C., S. C. Tsay, M. D. King, and J. R. Herman (2006), Deep blue retrievals of Asian aerosol properties during ACE-Asia, IEEE Trans. Geosci. Remote Sens., 44, 3180–3195.

Hu, L., D. B. Millet, M. J. Mohr, K. C. Wells, T. J. Griffis, and D. Helmig (2011), Sources and seasonality of atmospheric methanol based on tall tower measurements in the US Upper Midwest, Atmos. Chem. Phys., 11, 11145–11156.

Hu, L., D. B. Millet, S. Y. Kim, K. C. Wells, T. J. Griffis, E. V. Fischer, D. Helmig, J. Hueber, and A. J. Curtis (2013), North American acetone sources determined from tall tower measurements and inverse modeling, Atmos. Chem. Phys., 13, 3379–3392.

Hu, L., D. B. Millet, M. Baasandorj, T. J. Griffis, K. R. Travis, C. Tessum, J. Marshall, W. F. Reinhart, T. Mikoviny, M. Müller, A. Wisthaler, M. Graus, C. Warneke, and J. de Gouw (2014), Emissions of C6-C8 aromatic compounds in the United States: Constraints from tall tower and aircraft measurements, J. Geophys. Res., in revision.

Jaars, K., J. P. Beukes, P. G. van Zyl, A. D. Venter, M. Josipovic, J. J. Pienaar, V. Vakkari, H. Aaltonen, H. Laakso, M. Kulmala, P. Tiitta, A. Guenther, H. Hellén, L. Laakso, and H. Hakola (2014), Ambient aromatic hydrocarbon measurements at Welgegund, South Africa,

Atmos. Chem. Phys., 14(13), 7075–7089, doi:10.5194/acp-14-7075-2014.

Jacob, D. J. (1986), Chemistry of OH in remote clouds and its role in the production of formic acid and peroxymonosulfate, J. Geophys. Res., 91, 9807–9826.

Jiang, G., and J. D. Fast (2004), Modeling the effects of VOC and NO x emission sources on ozone formation in Houston during the TexAQS 2000 field campaign, Atmos. Environ., 38, 5071-5085, doi:10.1016/j.atmosenv.2004.06.012.

Johnson, D., M. E. Jenkin, K. Wirtz, and M. Martin-Reviejo (2005), Simulating the formation of secondary organic aerosol from the photooxidation of aromatic hydrocarbons, Environ. Chem., 2(1), 35–48, doi:10.1071/EN04079.

Jones, D. B. A., K. W. Bowman, P. I. Palmer, J. R. Worden, D. J. Jacob, R. N. Hoffman, I. Bey, and R. M. Yantosca (2003), Potential of observations from the Tropospheric Emission Spectrometer to constrain continental sources of carbon monoxide, J. Geophys. Res., 108(D24), 4789, doi: doi:10.1029/2003JD003702.

Jones, D. B. A., K. W. Bowman, J. A. Logan, C. L. Heald, J. Liu, M. Luo, J. Worden, and J. Drummond (2009), The zonal structure of tropical O_3 and CO as observed by the Tropospheric Emission Spectrometer in November 2004 – Part 1: Inverse modeling of CO emissions, Atmos. Chem. Phys., 9, 3547–3562, doi:10.5194/acp-9-3547-2009.

Karion, A., C. Sweeney, P. Tans, and T. Newberger (2010), AirCore: An Innovative Atmospheric Sampling System, J. Atmos. Oceanic Technol., 27, 1839–1853, doi:10.1175/2010JTECHA1448.1.

Keene, W. C., and J. N. Galloway (1984), Organic acidity in precipitation of North America, Atmos. Environ., 18, 2491–2497.

Keene, W. C., J. N. Galloway, and J. D. Holden (1983), Meassurement of weak organic acidity in precipitation from remote areas of the world, J. Geophys. Res., 88, 5122–5130.

Kim, S. Y., D. B. Millet, L. Hu, M. J. Mohr, T. J. Griffis, D. Wen, J. C. Lin, S. M. Miller, and M. Longo (2013), Constraints on carbon monoxide emissions based on tall tower measurements in the US Upper Midwest, Environ. Sci. Technol., 47, 8316–8324.

Kopacz, M., D. J. Jacob, J. A. Fisher, J. A. Logan, L. Zhang, I. A. Megretskaia, R. M. Yantosca, K. Singh, D. K. Henze, J. P. Burrows, M. Buchwitz, I. Khlystova, W. W. McMillan, J. C. Gille, D. P. Edwards, A. Eldering, V. Thouret, and P. Nedelec (2010), Global estimates of CO sources with high resolution by adjoint inversion of multiple satellite datasets (MOPITT, AIRS, SCIAMACHY, TES), Atmos. Chem. Phys., 10, 855–876, doi:10.5194/acp-10-855-2010.

Lamarque, J.-F., B. V. Khattatov, J. C. Gille, and G. P. Brasseur (1999), Assimilation of Measurement of Air Pollution from Space (MAPS) CO in a global three-dimensional model, J. Geophys. Res., 104, D21, 26,209–26,218.

Lamarque, J. F., D. T. Shindell, B. Josse, P. J. Young, I. Cionni, V. Eyring, D. Bergmann, P. Cameron-Smith, W. J. Collins, R. Doherty, S. Dalsoren, G. Faluvegi, G. Folberth, S. J. Ghan, L. W. Horowitz, Y. H. Lee, I. A. MacKenzie, T. Nagashima, V. Naik, D. Plummer, M. Righi, S. T. Rumbold, M. Schulz, R. B. Skeie, D. S. Stevenson, S. Strode, K. Sudo, S. Szopa, A. Voulgarakis, and G. Zeng (2013), The Atmospheric Chemistry and Climate Model Intercomparison Project (ACCMIP): overview and description of models, simulations and climate diagnostics, Geosci. Model Dev., 6(1), 179–206.

Le Breton, M., M. R. McGillen, J. B. A. Muller, A. Bacak, D. E. Shallcross, P. Xiao, L. G. Huey, D. Tanner, H. Coe, and C. J. Percival (2012), Airborne observations of formic acid using a chemical ionization mass spectrometer, Atmos. Meas. Tech., 5, 3029–3039.

Levy, R. C., L. A. Remer, S. Mattoo, E. F. Vermote, and Y. J. Kaufman (2007), Second-generation operational algorithm: Retrieval of aerosol properties over land from inversion of Moderate Resolution Imaging Spectroradiometer spectral reflectance, J. Geophys. Res., 112, D13211, doi:13210.11029/12006JD007811.

Liu, J., K. Bowman, M. Lee, D. Henze, N. Bousserez, H. Brix, G. J. Collatz, D.

Menemenlis, L. Ott, S. Pawson, D. Jones, and R. Nassar (2014), Carbon monitoring system flux estimation and attribution: impact of ACOS-GOSAT XCO2 sampling on the inference of terrestrial biospheric sources and sinks, Tellus B, 66(0), doi:http://dx.doi.org/10.3402/ tellusb.v66.22486.

Liu, Z., Y. Wang, D. Gu, C. Zhao, L. G. Huey, R. Stickel, J. Liao, M. Shao, T. Zhu, L. Zeng, S. C. Liu, C. C. Chang, A. Amoroso, and F. Costabile (2010), Evidence of reactive aromatics as a major source of peroxy acetyl nitrate over China, Environ. Sci. Technol., 44(18), 7017–7022, doi:10.1021/es1007966.

Liu, Z., Y. Wang, M. Vrekoussis, A. Richter, F. Wittrock, J. P. Burrows, M. Shao, C-C. Chang, S-C. Liu, H. Wang, and C. Chen (2012), Exploring the missing source of glyoxal (CHOCHO) over China, Geophys. Res. Lett., 39(10), L10812, doi:10.1029/2012gl051645.

Logan, J. A., I. Megretskaia, R. Nassar, L. T. Murray, L. Zhang, K. W. Bowman, H. M. Worden, and M. Luo (2008), Effects of the 2006 El Niño on tropospheric composition as revealed by data from the Tropospheric Emission Spectrometer (TES), Geophys. Res. Lett., 35, L03816, doi:10.1029/2007GL031698.

Luo, M., M. W. Shephard, K. E. Cady-Pereira, D. K. Henze, L. Zhu, J. O. Bash, R. W. Pinder, S. Capps, and J. Walker (2015), Satellite Observations of Tropospheric Ammonia and Carbon Monoxide: Global Distributions, Correlations and Comparisons to Model Simulations, accepted by Atmospheric Environment.

Martín-Reviejo, M., and K. Wirtz (2005), Is benzene a precursor for secondary organic aerosol?, Environ. Sci. Technol., 39(4), 1045–1054, doi:10.1021/es049802a.

McMillan, W. W., R. B. Pierce, L. C. Sparling, G. Osterman, K. McCann, M. L. Fischer, B. Rappenglück, R. Newsom, D. Turner, C. Kittaka, K. Evans, S. Biraud, B. Lefer, A. Andrews, and S. Oltmans (2010), An observational and modeling strategy to investigate the impact of remote sources on local air quality: A Houston, Texas, case study from the Second Texas Air Quality Study (TexAQS II), J. Geophys. Res., 115, D01301, doi:10.1029/2009JD011973.

Migliorini, S., C. Piccolo, and C. D. Rodgers (2008), Use of the information content in satellite measurements for an efficient interface to data assimilation, Mon. Wea. Rev., 136(7), 2633–2650.

Millet, D. B., M. Baasandorj, D. K. Farmer, J. A. Thornton, K. Baumann, P. Brophy, S. Chaliyakunnel, J. A. de Gouw, M. Graus, L. Hu, A. Koss, B. H. Lee, F. D. Lopez-Hilfiker, J. A. Neuman, F. Paulot, J. Peischl, I. B. Pollack, T. B. Ryerson, C. Warneke, B. J. Williams, and J. Xu (2015), A large and ubiquitous source of atmospheric formic acid, Atmos. Chem. Phys., submitted.

Moore, D. P., and J. J. Remedios (2010), Seasonality of Peroxyacetyl nitrate (PAN) in the upper troposphere and lower stratosphere using the MIPAS-E instrument, Atmos. Chem. Phys., 10(13), 6117–6128,10.5194/acp-10-6117-2010.

Myhre, G., D. Shindell, F.-M. Bréon, W. Collins, J. Fuglestvedt, J. Huang, D. Koch, J.-F. Lamarque, D. Lee, B. Mendoza, T. Nakajima, A. Robock, G. Stephens, T. Takemura, and H. Zhang (2014), Climate Change 2013: The Physical Science Basis. Contribution of Working Group I to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change, chapter Anthropogenic and Natural Radiative Forcing, pages 659–740. Cambridge University Press.

Nassar, R., D. B. A. Jones, S. S. Kulawik, J. R. Worden, K. W. Bowman, R. J. Andres, P. Suntharalingam, J. M. Chen, C. A. M. Brenninkmeijer, T. J. Schuck, T. J. Conway, and D. E. Worthy (2011), Inverse modeling of CO2 sources and sinks using satellite observations of CO2 from TES and surface flask measurements, Atmos. Phys., 11(12), 6029–6047, doi:10.5194/acp-11-6029-2011.

Ng, N. L., J. H. Kroll, A. W. H. Chan, P. S. Chhabra, R. C. Flagan, and J. H. Seinfeld (2007), Secondary organic aerosol formation from m-xylene, toluene, and benzene, Atmos. Chem. Phys., 7(14), 3909–3922, doi:10.5194/acp-7-3909-2007.

Paulot, F., D. Wunch, J. D. Crounse, G. C. Toon, D. B. Millet, P. F. DeCarlo, C. Vigouroux, N. M. Deutscher, G. G. Abad, J. Notholt, T. Warneke, J. W. Hannigan, C. Warneke, J. A. de Gouw, E. J. Dunlea, M. D. Mazière, D. W. T. Griffith, P. Bernath, J. L. Jimenez, and P. O. Wennberg (2011), Importance of secondary sources in the atmospheric budgets of formic and acetic acids, Atmos. Chem. Phys., 11, 1989–2013.

Payne, V. H., M. J. Alvarado, K. E. Cady-Pereira, J. R. Worden, S. S. Kulawik, and E. V. Fischer (2014), Satellite observations of peroxyacetyl nitrate from the Aura Tropospheric Emission Spectrometer, Atmos. Meas. Tech., 7, 3737–3749, doi:10.5194/amt-7-3737-2014.

Pierce, R. B., J. Al-Saadi, C. Kittaka, T. Schaack, A. Lenzen, K. Bowman, J. Szykman, A. Soja, T. Ryerson, A. M. Thompson, P. Bhartia, and G. A. Morris (2009), Impacts of background ozone production on Houston and Dallas, Texas, air quality during the Second Texas Air Quality Study field mission, J. Geophys. Res., 114, D00F09, doi:10.1029/2008JD011337

Pierce, R. B., T. Schaack, and A. Lenzen (2011), GOES Total Column Ozone Assimilation within the Community Multi-scale Air Quality Forecast Model, Joint Center for Satellite Data Assimilation Quarterly, No. 34, March 2011. (http://www.jcsda.noaa.gov/documents/newsletters/201103JCSDAQuarterly.pdf).

Pierangelo, C., A. Chédin, S. Heilliette, N. Jacquinet-Husson, and R. Armante (2004), Dust altitude and infrared optical depth from AIRS, Atmos. Chem. Phys., 4, 1813–1822.

Pierangelo, C., M. Mishchenko, Y. Balkanski, and A. Chédin (2005), Retrieving the effective radius of Saharan dust coarse mode from AIRS, Geophys. Res. Lett., 32, L20813.

Rinsland, C. P., C. Paton-Walsh, N. B. Jones, D. W. T. Griffith, A. Goldman, S. W. Wood, L. Chiou, and A. Meier (2005), High spectral resolution solar absorption measurements of ethylene (C_2H_4) in a forest fire smoke plume using HITRAN parameters: Tropospheric vertical profile retrieval, J. Quant. Spectrosc. Radiat. Transfer, 96, 301-309, doi:10.1016/j.jqsrt.2005.03.003.

Robichaud, A., and R. Ménard (2014), Multi-year objective analyses of warm season ground-level ozone and PM2.5 over North America using real-time observations and Canadian operational air quality models, Atmos. Chem. Phys., 14, 1769–1800.

Rodgers, C. D. (2000), Inverse Methods for Atmospheric Sounding: Theory and Practice, World Sci., Hackensack, N. J., 2000.

Rodgers, C. D., and B. J. Connor (2003), Intercomparison of remote sounding instruments, J. Geophys. Res., 108, 4116, doi:10.1029/2002JD002299.

Shephard, M.W., K. E. Cady-Pereira, M. Luo, D. K. Henze, R. W. Pinder, J. T. Walker, C. P. Rinsland, J. O. Bash, V. Payne, L. Clarisse (2011), TES Ammonia Retrieval Strategy and Global Observations of the Spatial and Seasonal Variability of Ammonia, Atmos. Chem. Phys., 11, 10743–10763, doi:10.5194/acp-11-10743-2011.

Shephard, M. W., and K. E. Cady-Pereira (2014), Cross-track Infrared Sounder (CrIS) Satellite Observations of Tropospheric Ammonia, Atmos. Meas. Tech. Discuss., 7, 11379–11413, doi:10.5194/amtd-7-11379-2014.

Shindell, D., G. Faluvegi, L. Nazarenko, K. Bowman, J.-F. Lamarque, A. Voulgarakis, G. A. Schmidt, O. Pechony, and R. Ruedy (2013a), Attribution of historical ozone forcing to anthropogenic emissions, Nature Clim. Change, 3(6), 567–570.

Shindell, D. T., O. Pechony, A. Voulgarakis, G. Faluvegi, L. Nazarenko, J. F. Lamarque, K. Bowman, G. Milly, B. Kovari, R. Ruedy, and G. A. Schmidt (2013b), Interactive ozone and methane chemistry in GISS-E2 historical and future climate simulations, Atmos. 13(5), 2653–2689, doi:10.5194/acp-13-2653-2013.

Simpson, I. J., M. P. Sulbaek Andersen, S. Meinardi, L. Bruhwiler, N. J. Blake, D. Helmig, F. S. Rowland, and D. R. Blake (2012), Long-term decline of global atmospheric ethane concentrations and implications for methane, Nature, 488, 490-494, doi:10.1016/S1352-2310(02)00302-3.

Singh, H. B. (1987), Reactive nitrogen in the troposphere: chemistry and transport of

NO_x and PAN, Environmental Science and Technology, 21, 320–327.

Stavrakou, T., A. Guenther, A. Razavi, L. Clarisse, C. Clerbaux, P. F. Coheur, D. Hurtmans, F. Karagulian, M. De Mazière, C. Vigouroux, C. Amelynck, N. Schoon, Q. Laffineur, B. Heinesch, M. Aubinet, C. Rinsland, and J. F. Müller (2011), First space-based derivation of the global atmospheric methanol emission fluxes, Atmos. Chem. Phys., 11, 4873–4898.

Stavrakou, T., J.-F. Müller, J. Peeters, A. Razavi, L. Clarisse, C. Clerbaux, P.-F. Coheur, D. Hurtmans, M.D. Mazière, C. Vigouroux, N.M. Deutscher, D.W.T. Griffith, N. Jones, and C. Paton-Walsh (2012), Satellite evidence for a large source of formic acid from boreal and tropical forests, Nature Geosci., 5, 26–30.

Strow, L. L., W. Blackwell, E. Fishbein, B. Lambrigtsen, and H. Revercomb (2013), NPP Sounding Group Evaluation Report, available at http://npp.gsfc.nasa.gov/DEW_NPP_reports/Sounder%20%28ATMS%20&%20CrIS%29%20Products%20Report%20%28Apr-10-2013%29.pdf.

Tereszchuk, K. A., D. P. Moore, J. J. Harrison, D. Boone, M. Park, J. J. Remedios, W. J. Randel, and P. F. Bernath (2013), Observations, of peroxyacetyl nitrate (PAN) in the upper troposphere by the Atmospheric Chemistry Experiment-Fourier Transform Spectrometer (ACE-FTS), Atmos. Chem. Phys., 13, 5601–5613.

Thompson, A.M., J. C. Witte, R. D. McPeters, S. J. Oltmans, F. J. Schmidlin, J. A. Logan, M. Fujiwara, V. W. J. H. Kirchhoff, F. Posny, G. J. R. Coetzee, B. Hoegger, S. Kawakami, T. Ogawa, B. J. Johnson, H. Vömel and G. Labow (2003), Southern Hemisphere Additional Ozonesondes (SHADOZ) 1998-2000 tropical ozone climatology 1. Comparison with Total Ozone Mapping Spectrometer (TOMS) and ground-based measurements, J. Geophys. Res., 108, 8238, doi:10.1029/2001JD000967.

Thompson, A.M., J. C. Witte, S. J. Oltmans, F. J. Schmidlin, J. A. Logan, M. Fujiwara, V. W. J. H. Kirchhoff, F. Posny, G. J. R. Coetzee, B. Hoegger, S. Kawakami, T. Ogawa, J. P. F. Fortuin, and H. M. Kelder (2003), Southern Hemisphere Additional Ozonesondes (SHADOZ) 1998-2000 tropical ozone climatology 2. Tropospheric variability and the zonal wave-one, J. Geophys. Res., 108, 8241, doi:10.1029/2002JD002241.

Thompson, A.M., J.C. Witte, H.G.J. Smit, S.J. Oltmans, B.J. Johnson, V.W.J H. Kirchhoff, and F.J. Schmidlin (2007), Southern Hemisphere Additional Ozonesondes (SHADOZ) 1998-2004 tropical ozone climatology: 3. Instrumentation, station-to-station variability, and evaluation with simulated flight profiles, J. Geophys. Res., 112, D03304, doi:10.1029/2005JD007042.

Torres, O., A. Tanskanen, B. Veihelmann, C. Ahn, R. Braak, P. K. Bhartia, P. Veefkind, and P. Levelt (2007), Aerosols and surface UV products from Ozone Monitoring Instrument observations: An overview, J. Geophys. Res., 112, D24S47, doi:10.1029/2007JD008809.

Wecht, K. J., D. J. Jacob, S. C. Wofsy, E. A. Kort, J. R. Worden, S. S. Kulawik, D. K. Henze, M. Kopacz, and V. H. Payne (2012), Validation of TES methane with HIPPO aircraft observations: implications for inverse modeling of methane sources, Atmos. Chem. Phys., 12, 1823–1832, doi:10.5194/acp-12-1823-2012.

Wells, K. C., and D. B. Millet (2014), Satellite-derived constraints on northern temperate hydrocarbon and CO emissions and the anthropogenic versus biogenic source of CO, presented at the 2014 Goldschmidt Conference, Sacramento, CA.

Wells, K. C., D. B. Millet, L. Hu, K. E. Cady-Pereira, Y. Xiao, M. W. Shephard, C. L. Clerbaux, L. Clarisse, P.-F. Coheur, E. C. Apel, J. de Gouw, C. Warneke, H. B. Singh, A. Goldstein, and B. C. Sive (2012), Tropospheric methanol observations from space: retrieval evaluation and constraints on the seasonality of biogenic emissions, Atmos. Chem. Phys., 12, 5897–5912, doi:10.5194/acp-12-5897-2012.

Wells, K. C., D. B. Millet, K. E. Cady-Pereira, M. W. Shephard, D. K. Henze, N. Bousserez, E. C. Apel, J. de Gouw, C. Warneke, and H. B. Singh (2014), Quantifying global terrestrial methanol emissions using observations from the TES satellite sensor, Atmos. Chem. Phys., 14, 2555–2570.

Worden, H., R. Beer, and C. Rinsland (1997), Airborne infrared spectroscopy of 1994 western wildfires, J. Geophys. Res., 102(D1), 1287.

Worden, H. M., J. A. Logan, J. R. Worden, R. Beer, K. Bowman, S. A. Clough, A. Eldering, B. M. Fisher, M. R. Gunson, R. L. Herman, S. S. Kulawik, M. C. Lampel, M. Luo, I. A. Megretskaia, G. B. Osterman, and M. Shephard (2007), Comparisons of Tropospheric Emission Spectrometer (TES) ozone profiles to ozonesondes: methods and initial results, J. Geophys. Res.-Atmospheres, 112, D03309, doi:10.1029/2006JD007258.

Worden, H. M., K. W. Bowman, J. R. Worden, A. Eldering, and R. Beer (2008), Satellite measurements of the clear-sky greenhouse effect from tropospheric ozone, Nature Geosci, 1(5), 305–308.

Worden, H. M., K. Bowman, S. Kulawik, and A. Aghedo (2011), Sensitivity of outgoing longwave radiative flux to the global vertical distribution of ozone characterized by instantaneous radiative kernels from Aura-TES, J. Atmos., doi:10.1029/2010JD015101.

Worden, H. M., M. N. Deeter, C. Frankenberg, M. George, F. Nichitiu, J. Worden, I. Aben, K. W. Bowman, C. Clerbaux, P. F. Coheur, A. T. J. de Laat, R. Detweiler, J. Drummond, D. P. Edwards, J. C. Gille, D. Hurtmans, M. Luo, S. Martínez-Alonso, S. Massie, G. Pfister, and J. X. Warner (2013a), Decadal record of satellite carbon monoxide observations, Atmos. Chem. Phys., 13, 837–850, doi:10.5194/acp-13-837-2013.

Worden, H. M., D. P. Edwards, M. N. Deeter, D. Fu, S. S. Kulawik, J. R. Worden, and A. Arellano (2013b), Averaging kernel prediction from atmospheric and surface state parameters based on multiple regression for nadir-viewing satellite measurements of carbon monoxide and ozone, Atmos. Meas. Tech., 6, 1633–1646, doi:10.5194/amt-6-1633-2013.

Worden, J., Z. Jiang, D. Jones, M. Alvarado, K. Bowman, C. Frankenberg, E. Kort, S. Kulawik, M. Lee, J. Liu, V. Payne, K. Wecht, and H. Worden (2013a), El Niño, the 2006 Indonesian peat fires, and the distribution of atmospheric methane, Geophys. Res. Lett., 40, 4938–4943, doi:10.1002/grl.50937.

Worden, J., K. Wecht, C. Frankenberg, M. Alvarado, K. Bowman, E. Kort, S. Kulawik, M. Lee, V. Payne, and H. Worden (2013b), CH_4 and CO distributions over tropical fires during October 2006 as observed by the Aura TES satellite instrument and modeled by GEOS-Chem, Atmos. Chem. Phys., 13, 3679–3692, doi:10.5194/acp-13-3679-2013.

Xiao, Y., D. J. Jacob, and S. Turquety (2007), Atmospheric acetylene and its relationship with CO as an indicator of air mass age, J. Geophys. Res., 112, D12305, doi:10.1029/2006JD008268.

Xiao, Y., J. A. Logan, D. J. Jacob, R. C. Hudman, R. Yantosca, and D. R. Blake (2008), Global budget of ethane and regional constraints on US sources, J. Geophys. Res., 113, D21306, doi:10.1029/2007JD009415.

Xue, L. K., T. Wang, J. Gao, A. J. Ding, X. H. Zhou, D. R. Blake, X. F. Wang, S. M. Saunders, S. J. Fan, H. C. Zuo, Q. Z. Zhang, and W. X. Wang (2014), Ground-level ozone in four Chinese cities: precursors, regional transport and heterogeneous processes, Atmos. Chem. Phys. Discuss., 14(14), 20767–20803, doi:10.5194/acpd-14-20767-2014.

Young, P. J., A. T. Archibald, K. W. Bowman, J. F. Lamarque, V. Naik, D. S. Stevenson, S. Tilmes, A. Voulgarakis, O. Wild, D. Bergmann, P. Cameron-Smith, I. Cionni, W. J. Collins, S. B. Dalsøren, R. M. Doherty, V. Eyring, G. Faluvegi, L. W. Horowitz, B. Josse, Y. Lee, I. A. MacKenzie, T. Nagashima, D. A. Plummer, M. Righi, S. T. Rumbold, R. B. Skeie, D. T. Shindell, S. A. Strode, K. Sudo, S. Szopa, and G. Zeng (2013), Pre-industrial to end 21st century projections of tropospheric ozone from the Atmospheric Chemistry and Climate Model Intercomparison Project (ACCMIP), Atmos. Chem. Phys., 13(4), 2063–2090, doi:10.5194/acp-13-2063-2013.

Zavyalov, V., M. Esplin, D. Scott, B. Esplin, G. Bingham, E. Hoffman, C. Lietzke, J. Predina, R. Frain, L. Suwinski, Y. Han, C. Major, B. Graham, and L. Phillips (2013), Noise performance of the CrIS instrument, J. Geophys. Res. Atmos., 118, 13,108–13,120, doi:10.1002/2013JD020457.

Zhang, L., D. Jacob, K. Bowman, J. A. Logan, S. Turquety, R. C. Hudman, Q. Li, R. Beer, H. Worden, J. Worden, C. P. Rinsland, S. S. Kulawik, M. C. Lampel, M. W. Shephard, B. M. Fisher, A. Eldering, and M. Avery (2006), Ozone-CO correlations determined by the TES satellite instrument in continental outflow regions, Geophys. Res. Lett., 33, L18804, doi:10.1029/2006GL026399.

Zhang, L., D. J. Jacob, K. F. Boersma, D. A. Jaffe, J. R. Olson, K. W. Bowman, J. R. Worden, A. M. Thompson, M. A. Avery, R. C. Cohen, J. E. Dibb, F. M. Flock, H. E. Fuelberg, L. G. Huey, W. W. McMillan, H. B. Singh, and A. J. Weinheimer (2008), Transpacific transport of ozone pollution and the effect of recent Asian emission increases on air quality in North America: an integrated analysis using satellite, aircraft, ozonesonde, and surface observations, Atmospheric Chemistry and Physics, 8(20), 6117–6136.

Zhu, L., D. K. Henze, K. E. Cady-Pereira, M. W. Shephard, M. Luo, R. W. Pinder, J. O. Bash, and G.-R. Jeong (2013), Constraining US ammonia emissions using TES remote sensing observations and the GEOS-Chem adjoint model, J. Geophys. Res. Atmos., 118, doi:10.1002/jgrd.50166.

9 Glossary of Acronyms

ACE-FTS: Atmospheric Chemistry Experiment – Fourier Transform Spectrometer

AER: Atmospheric and Environmental Research, Incorporated

AERI: Atmospheric Emitted Radiance Interferometer

AEROSE: AErosols and Ocean Science Expeditions

AES: Airborne Emission Spectrometer

AIRS: Atmospheric InfraRed Sounder

AJAX: Alpha Jet Atmospheric eXperiment

AK: Averaging Kernel

AR5: Fifth Assessment Report (from the IPCC)

ARCTAS-B: Arctic Research of the Composition of the Troposphere from Aircraft and Satellites

ARL: Air Resources Laboratory (at NOAA)

ATom: Atmospheric Tomography mission

ATTREX: Airborne Tropical TRopopause EXperiment

AM3: The atmospheric component of the GFDL coupled climate model CM3.

BAO: Boulder Atmospheric Observatory

BTEX: Benzene, Toluene, Ethylbenzene, and Xylenes

CAM-Chem: Community Atmosphere Model with Chemistry

CARIBIC: Civil Aircraft for the Regular Investigation of the atmosphere Based on an Instrument Container

CAST: Coordinated Airborne Studies in the Tropics

C-IFS: Integrated Forecasting System

CLASS: Comprehensive Large Array-data Stewardship System

CMAQ Model: Community Multi-scale Air Quality Model

CMS: Carbon Monitoring System

CONTRAIL: Comprehensive Observation Network for TRace gases by AIrLiner

CPO: Climate Program Office (at NOAA)

CrIS: Cross-track Infrared Sounder

CSAR: Center for Satellite Applications and Research

CSD: Chemical Sciences Division (at NOAA ESRL)

CSPP: Community Satellite Processing Package

CSU: Colorado State University

DISCOVER-AQ: Deriving Information on Surface conditions from Column and Vertically Resolved Observations Relevant to Air Quality

DOD: Department of Defense

ECMWF: European Center for Medium-range Weather Forecasting

EDR: Environmental Data Record (associated with NUCAPS)

EOS: Earth Observing System

ESPO: Earth Science Program Office (at NASA)

ESRL: Earth System Research Laboratory (at NOAA)

EUMETSAT: EUropean organisation for the exploitation of METeorological SATellites

FIREX: Fire Influence on Regional and global environments EXperiment

FLEXPART: FLEXible PARTicle dispersion model

FRAPPÉ: Front Range Air Pollution and Photochemistry Éxperiment

FTIR: Fourier Transform InfraRed

GCOS: Global Climate Observing System

GEM-MACH: Global Environmental Multi-scale – Modeling Air quality and CHemistry

GEOS-5: Goddard Earth Observing System model

GEOS-Chem: Goddard Earth Observing System model with Chemistry

GFDL: Geophysical Fluid Dynamics Laboratory (at NOAA)

GFS: Global Forecast System

GHOST: GreenHouse Observations of the Stratosphere and Troposphere

GISS: Goddard Institute for Space Studies (at NASA GSFC)

GMD: Global Monitoring Division (at NOAA ESRL)

GOES: Geostationary Operational Environmental Satellite

GRUAN: GCOS Reference Upper-Air Network

GSFC: Goddard Space Flight Center (at NASA)

HAP: Hazardous Air Pollutant

HSRL: High Spectral Resolution LiDAR (Light Detection And Ranging)

IAGOS: In-service Aircraft for the Global Observing System

IASI: Infrared Atmospheric Sounding Interferometer

IASI-NG: New Generation of Infrared Atmospheric Sounding Interferometer

IPCC: Intergovernmental Panel on Climate Change (associated with the World Meteorological Organization and the United Nations Environment Programme)

IRK: Instantaneous Radiative Kernel

JPL: Jet Propulsion Laboratory (at NASA)

JPSS-2: Joint Polar Satellite System

MACC-III: Monitoring Atmospheric Composition and Climate

MLS: Microwave Limb Sounder

MIPAS: Michelson Interferometer for Passive Atmospheric Sounding

MODIS: Moderate Resolution Imaging Spectrometer

MOPITT: Measurements Of Pollution In The Troposphere

MOZAIC: Measurement of OZone and water vapor by AIrbus in-service aircraft

MOZART-4: Model for OZone And Related chemical Tracers

MRI: Meteorological Research Institute (in Japan)

NAM-CMAQ: North American Model of the Community Multi-scale Air Quality Model

NASA: National Aeronautics and Space Administration

NCAR: National Center for Atmospheric Research

NDACC: Network for the Detection of Atmospheric Composition Change

NERC: Natural Environment Research Council

NESDIS: National Environmental Satellite, Data, and Information Service (at NOAA)

NIES: National Institute for Environmental Studies (in Japan)

NMVOC: Non-Methane Volatile Organic Compound

NOAA: National Oceanic and Atmospheric Administration

NOGAPS: Navy Operational Global Atmospheric Prediction System

NSF: National Science Foundation

NUCAPS: NOAA Unique CrIS/ATMS Processing System

NWS: National Weather Service (at NOAA)

OCO-2: Orbiting Carbon Observatory

OMI: Ozone Monitoring Instrument

OMPS: Ozone Mapping Profiler Suite

PAN: PeroxyAcetylNitrate

RAQMS: Real-time Air Quality Modeling System

RR-Chem: Rapid Refresh with Chemistry modeling system

SEACIONS: SouthEast American Consortium for Intensive Ozonesonde Network Study

SEAC4RS: Studies of Emissions and Atmospheric Composition, Clouds and Climate Coupling by Regional Surveys

SENEX: SouthEast NEXus of air quality and climate campaign

SHADOZ: Southern Hemisphere ADditional OZonesondes

SOAS: Southern Oxidant and Aerosol Study

SONGNEX: Shale Oil and Natural Gas NEXus of air quality and climate campaign

SSEC/CIMSS: Space Science and Engineering Center/Cooperative Institute for Meteorological Satellite Studies (at UW)

STAR: Center for SaTellite Applications and Research (at NOAA NESDIS)

STC: Science and Technology Corporation

Suomi-NPP: Suomi National Polar-orbiting Partnership

SVD: Singular Value Decomposition

TCCON: Total Column Carbon Observing Network

TES: Tropospheric Emission Spectrometer

TIR: Thermal InfraRed

TOA: Top-Of-Atmosphere

UAS: Unmanned Aircraft Systems

UAV: Unpiloted Aerial Vehicle

UCATS: UAS Chromatograph for Atmospheric Trace Species

UMBC: University of Maryland-Baltimore County

UW: University of Wisconsin-Madison

VALAR: VALidation ARchive

VOC: Volatile Organic Compound

WINTER: Wintertime INvestigation of Transport, Emissions, and Reactivity

WRF-Chem: Weather Research and Forecasting with Chemistry model

Notice from NOAA

The CrIS instrument is carefully loaded into the JPSS spacecraft.
Photo Credit: Ball Aerospace & Technologies Corp.

Advancing Atmospheric Chemistry Through the Use of Satellite Observations from the Cross-track Infrared Sounder (CrIS)

CrIS Atmospheric Chemistry Data User's Workshop Report

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