NOAA JPSS Science Team Meeting

Trace gas session

Antonia Gambacorta and Monika Kopacz Co-conveners

August 18, 2017

Auditorium: Trace Gases

Time	Presentations / Topics	Speaker	Affiliation
0830 - 0900	Night Vision: Illuminating the Capabilities of the VIIRS Day/Night Band Auditorium	Curtis Seaman	CIRA
0915 - 1700	Trace Gases Chairs: Antonia Gambacorta and Monika Kopacz Auditorium	es tonia Gambacorta and Monika Kopacz 1	
0915 - 0930	Opening Remarks	Antonia Gambacorta; Monika Kopacz	STC;CPO
0930 - 0950	Status of the NUCAPS Full Spectral Resolution trace gas products	I Spectral Resolution trace gas products Antonia Gambacorta	
0950 - 1010	Status of NUCAPS Full Spectral Resolution Trace Gas EDR Validation	Nick Nalli	IMSG
1010 - 1030	Forward Model Improvements: Present and Future	Larrabee Strow	UMBC
1030 - 1100	Break		
1100 - 1120	What are NUCAPS trace gas retrievals good for?	Nadia Smith	
1120 - 1140	Evaluating NUCAPS CH4 and CO	Greg Frost	NOAA/ESRL
1140 - 1200	Recent Improvements in NUCAPS CH4 retrievals using CrIS FSR data	Xiaozhen Xiong	
1200 - 1330	Lunch		
1330 - 1350	Ising Ammonia Retrievals from the Cross-track Infrared Sounder to mprove Emission Inventories and Models.		AER, Inc.
1350 - 1410	Increased atmospheric ammonia over the world's major agricultural areas detected from space	major agricultural Juying Warner	
1410 - 1430	Multi-species, Multi-Spectral, Multi-Satellite retrievals of trace gases	llite retrievals of trace gases Vivienne Payne	
1430 - 1450	Full-chemistry Vog Forecasting over Hawaii	Youhua Tang	ARL
1450 - 1500	3reak		
1500 - 1520	Smithsonian Astrophysical Observatory OMPS Nadir Mapper formaldehyde retrievals	Gonzalo Gonzalez Abad	Harvard
1520 - 1540	Monitoring Atmospheric NO2 and SO2 from Space: Half a Decade of Suomi NPP OMPS Global Observation	Kai Yang	NASA
1540 - 1600	Development of Multi-sensor JPSS SO2 Products for Volcanic Cloud Monitoring	Mike Pavolonis	STAR
1600 - 1610	Closing Remarks	Monika Kopacz; Antonia Gambacorta CPO; STC	

NOAA (OAR/CPO/AC4) effort so far

- **2013**: FY13 FFO funded ammonia product development and validation
- 2014: FY14 FFO funded further development of ammonia product; CrIS workshop gathers potential (research) users
- 2015: FY15 FFO funded ammonia product application in GFDL Earth System Model; CrIS workshop report released
- 2016-17: FY16 FFO funded CrIS/OMPS ozone product development
- 2017: FY18 FFO solicits for new (BVOC) product development – 5 relevant proposals

How did we contribute? Mostly through FFO...

More progress: CrIS workshop recommendations (2015)

Scientific community uses TIR satellite observation, so far provided by NASA and EUMETSAT from **MOPITT, TES, AIRS and IASI**. All are past expiration and there are no plans to replace them.

Recommendation 1: Need data

• Provide calibrated radiances Level 1b data at full spectral resolution.

Recommendation 2: Special needs for atmospheric chemistry

- A. Provide reduced file size (like TES "lite) with retrievals for individual trace gases and their observation operators at a reduced vertical resolution.
- B. Provide essential information: a priori, averaging kernels, estimated retrieval error.
- C. Allow rapid multi-file download from CLASS

Recommendation 3: Validation

- A. Coordinate validation with upcoming field campaigns (e.g. FIREX)
- B. More frequent ESRL flights to validate trace gases
- C. Plan additional field campaigns with retrieval and user communities

Recommendation 4: Future

- A. Explore the possibility of new species/products
- B. Close spectral gap
- C. Reduce noise and increase resolution for future instruments

Most apply to all of JPSS!



What are the applications?

- Improved understanding of atmospheric composition
- NOAA Climate/Earth System Model (GFDL) development and validation
- Air quality forecasting
- NGGPS
- Monitoring of air pollution and greenhouse gases

Priorities??? Workshops needed??

Air quality services: Can we keep up with Copernicus?





"The service provides nearreal-time analysis and 4-day forecasts, as well as reanalysis, of the European air quality, thus enabling a permanent assessment of the air we breathe."

http://atmosphere.copernic us.eu/services/air-qualityatmospheric-composition

Figure courtesy of Mark Parrington and Vincent-Henri Peuch, ECMWF

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Antonia Gambacorta ⁽¹⁾, Nick Nalli ⁽²⁾, Flavio Iturbide-Sanchez⁽²⁾, Changyi Tan⁽²⁾, Kexin Zhang⁽²⁾, Xiaozhen Xiong⁽²⁾, Bomin Sun⁽²⁾, Mike Wilson⁽²⁾, Tish Suillard⁽²⁾, Tom King⁽²⁾, Chris Barnet⁽¹⁾, Ahsley Wheleer⁽¹⁾, Nadia Smith⁽¹⁾, Larrabee Strow⁽⁴⁾, Tony Reale⁽³⁾, Mark Liu⁽³⁾, Lihang Zhou⁽³⁾, AK Sharma⁽³⁾, Walter Wolf⁽³⁾, Mitch Goldberg⁽⁵⁾

2017 JPSS Annual Meeting – Trace Gas Session

¹STC; ² IMSG^{; 3} NOAA/NESDIS/STAR; ⁴UMBC; ⁵NOAA JPSS



Outline of this talk

Part I.

Introduction on the NUCAPS system

Part II.

Overview of the NUCAPS Full Spectral Resolution (FSR) upgrades relevant to trace gas retrievals

- SARTA RTA upgrades and bias corrections
- CrIS FSR trace gases channel selection

Part III.

Current activities, future plans



N as in NUCAPS

NOAA	NOAA's mandate: ensuring highest computational efficiency and state of art inversion methods to maximize utilization of large volumes of data for a weather ready nation		
Unique	A mathematically sound, globally applicable (land/ocean, day/night, all season, all sky, TOA-surface) hyperspectral retrieval code		
Combined	that can fully exploit all available satellite assets: infrared, microwave, visible		
Atmospheric	to generate a full suite of retrieval products: cloud cleared radiances, skin temperature, vertical profiles of temperature, water vapor, O3, CO, CH4, HNO3, N2O, SO2, CO2 (future: HN3)		
Processing	by the use of a modular design compatible with multiple platforms: Aqua, MetOp, SNPP, JPSS, EPS-SG		
System	NUCAPS has been running operationally at NOAA since 2004. it is now in AWIPS II. It has been installed in CSPP DB.		



Nominal vs Full Spectral Resolution CrIS

- The Cross-Track Infrared Sounder (CrIS) is a Fourier spectrometer covering the longwave (655-1095 cm⁻¹, "LW"), midwave (1210-1750 cm⁻¹, "MW"), and shortwave (2155-2550 cm⁻¹, "SW") infrared spectral regions.
- Past operations (NUCAPS Phase 1-3):
 - Maximum geometrical path L of 0.8 cm (LW), 0.4 cm (MW) and 0.2 cm (SW)
 - Nyquist spectral sampling (1/2L): 0.625 cm⁻¹, 1.25 cm⁻¹ and 2.5 cm⁻¹
- Experimental since 2013 Operational in August 2017 (NUCAPS Phase 4):
 - Maximum geometrical path *L* of 0.8 cm in all three bands
 - Nyquist spectral sampling (1/2L): 0.625 cm⁻¹ in all three bands

CrIS Full Spectral Resolution (FSR) SARTA Rapid Transmittance Algorithm (RTA)

Upgrades in the CrIS FSR SARTA RTA (L. Strow's talk in the today's session)

- CrIS high-resolution ILS
- HITRAN 2012 (vs 2008 in original CrIS RTA)
- LBLRTM Line Mixing for CO2 and CH4, H2O continuum
- UMBC line-by-line for water vapor
- Improved reflected thermal component for high secant angles
- Tested on 750+ profiles (from ECMWF selected subset), regressed on 49 profiles
- Error covariance estimates available from 750+ profile testing



CrIS FSR SARTA bias tuning and sdev



CH4 and CO2 profiles from JAMSTEC atmospheric chemistry-transport model (ACTM) as truth. CO profiles from MOPITT retrieval as truth. Selection of clear CrIS FOVs was performed using collocated VIIRS cloud mask IPs. (1) only confident clear pixels; (2) satellite view angle less than +/-30 degrees; (3) set multi-thresholds to screen out outliners.



Channel Selection Methods: two schools of thoughts

Jacobians method aka "Physical Approach"

- Selection methodology metrics:
 - Channel spectral purity
- Current operational users (to cite a few)
 - AIRS science team (1,3)
 - NOAA (AIRS, IASI, CrIS) ^(1,2)
 - ECMWF (IASI)⁽⁴⁾
 - Meteo UK (IASI) ⁽⁴⁾
 - Meteo France (IASI)⁽⁴⁾
 - LATMOS (AIRS, IASI, CrIS) ⁽⁵⁾
 - ULB (AIRS, IASI, CrIS)⁽⁵⁾
- List of references
 - (1) Susskind, Barnet, Blaisdell, IEEE 2003
 - (2) Gambacorta and Barnet, IEEE 2013;
 - (3) Susskind, Blaisdell, Iredell, JARS, 2014
 - (4) Martinet, Levananat, Fourrie, Gambacorta, 2014
 - (5) Crevoisier, Chedin, Scott, QJRM, 2003

Rodgers Method

- Selection methodology metrics:
 - Channel information content
- Current operational users (to cite a few)
 - ECMWF ^(1,2,3,4)
 - Meteo UK ^(1,2,3,4)
 - Meteo France ^(1,2,3,4)

- List of references
 - (1) Rodgers, 1997
 - (2) Fourrie *et al*. 2002;
 - (3) Rabier *et al.,* 2002
 - (4) Collard and McNally, 2007



Physical Method vs Rodgers Method

Jacobians or Physical method

- A physically-based methodology where channels are selected upon their spectral properties.
- For each atmospheric species, we perform a spectral sensitivity analysis and retain the spectrally purest channels and reject channels carrying confounding signals.
- Other than spectral purity, priority is given to vertical sensitivity properties, low instrumental noise and RTA errors.
- The method is algorithm independent in that both simultaneous and sequential inversion algorithms benefit from channels that can discriminate between atmospheric species. Details to be explained ahead.

Rodgers method

- Follows a statistical iterative approach where channels are incrementally added after being tested for increased degrees of freedom.
- This methodology is more suited for simultaneous optimal estimation retrieval techniques.
- Can be automated by establishing fixed thresholds.

Both methods:

• a constant channel selection is normally used, which is derived as an average from multiple optimal selections computed over different geophysical regimes (polar, mid latitudes, tropical, land, ocean, desert).



CrIS FSR Channel Selection



Brightness temperature difference (ΔBT) terms represent the sensitivity of each channel to a given perturbation species and are indicative of the degree of *"spectral purity"* of each channel.

- •For each atmospheric species, we select channels with:
 - the highest degree of spectral purity (the highest sensitivity to the species of interest and the lowest sensitivity to all other interfering species).
 - the lowest noise sources (NEDT, calibration & apodization corr., RTA errors)
 - unique spectral features (to capture atmospheric variability, maximize vertical resolution)

REF: A. Gambacorta and C. Barnet., Methodology and information content of the NOAA NESDIS operational channel selection for the Cross-Track Infrared Sounder (CrIS), IEEE, Vol. 51, Issue 6, 2013



Why do we use the Jacobian method

- NUCAPS required list of retrieval products (all sky, all seasons, all surface types)
 - Cloud cleared radiances
 - Cloud top pressure and fraction
 - Surface temperature
 - Vertical temperature
 - Water vapor
 - Trace gases: O_3 , CH_4 , CO, CO_2 , SO_2 , N_2O , HNO_3
- Future candidates:
 - NH₃ (Ammonia), HCO₂H (Formic Acid), CH₃COOONO₂ ("PAN")
- A "trace gas" is a gas which makes up less than 1% of the volume of the Earth's atmosphere.
- Trace gas radiative signals are in the range of the instrument noise.
- Most channels are largely contaminated by clouds, temperature and water vapor signals.
- <u>Answer</u>: Spectral purity is essential to improve signal to noise for the retrieval of the full list of NUCAPS required products, particularly for trace gases, under all sky conditions.
- This methodology, being *physically based*, is applicable to *ALL* retrieval schemes. It is particularly suited for sequential retrieval approaches. See next slide.

REF: A. Gambacorta and C. Barnet., Methodology and information content of the NOAA NESDIS operational channel selection for the Cross-Track Infrared Sounder (CrIS), IEEE, Vol. 51, Issue 6, 2013



Why do we use the Jacobian method

Summary of current NUCAPS retrieval products

gas	Range (cm ⁻¹)	Precision	d.o.f.	Interfering Gases
т	650-800 2375-2395	1K/km	6-10	H2O,O3,N2O emissivity
H ₂ O	1200-1600	15%	4-6	CH4, HNO3
0 ₃	1025-1050	10%	1+	H2O, emissivity
со	2080-2200	15%	≈1	H2O,N2O
CH4	1250-1370	1.5%	≈1	H2O,HNO3,N2O
CO ₂	680-795 2375-2395	0.5%	≈1	H2O,O3 T(p)
<u>Volcanic</u> SO ₂	1340-1380	50% ??	< 1	H2O,HNO3
HNO ₃	860-920 1320-1330	50% ??	< 1	emissivity H2O,CH4,N2O
N ₂ O	1250-1315 2180-2250	5% ??	< 1	H2O H2O,CO
CFCl ₃ (F11)	830-860	20%	-	emissivity
CF ₂ Cl (F12)	900-940	20%	-	emissivity
CCl ₄	790-805	50%	-	emissivity

Potential additions



 Sequential OE (solves each state variable separately) vs simultaneous OE (solves all parameters simultaneously) approach

$$egin{aligned} R_n^{obs} &- R_n(ec{X}) \simeq K_{n,i}^1 \cdot \Delta ec{T_i} + e_n \ e_n &= K_{n,i}^2 \cdot \delta ec{q_i} \ &+ K_{n,i}^3 \cdot \delta ec{O_i} \ &+ K_{n,i}^4 \cdot \delta ec{C} O_i \ &+ \ldots + \epsilon_n \end{aligned}$$

- Careful analysis of the physical spectrum will show that many components are physically separable (spectral derivatives are unique).
- Select channels within each step with large K and small e_n
- This makes the solution more linear with respect to the simultaneous OE approach.
- State matrices are small and covariance matrices of the channel subsets are quite small. This has significant implications for operational execution time.

NUCAPS Operational FSR CrIS channel selection (610 channels)





August 2013: Preliminary demonstration of FSR NUCAPS CO (top) vsNSR NUCAPS CO (bottom) using 5 test FSR orbits and ~2008 FSR RTANUCAPS CO retrieval (~450mb)NUCAPS CO DOF



- The higher information content enables a larger departure from the a priori, hence the increased spatial variability observed in the high spectral resolution map (top left) compared to the low resolution (bottom left).
- August 2013: this was a demonstration experiment in support for the need of high spectral resolution CrIS measurements using 5 experimental orbits from March 2013. Top is FSR NUCAPS; Bottom is NSR NUCAPS.

Ref.: Gambacorta et al., "An experiment using CrIS high spectral resolution measurement for trace gas retrievals: CO retrieval impact study", IEEE Transactions on Geoscience and Remote Sensing Letters, 2014.



December 2016: Preliminary demonstration of FSR NUCAPS CO (top) vs NSR NUCAPS CO (bottom) using Operational FSR RTA and Chn. Selection NUCAPS CO retrieval (~450mb) NUCAPS CO DOF



TOP: FSR NUCAPS/CLIMCAPS CO retrieval results (focus day 2015-02-17) **BOTTOM: NSR** NUCAPS/CLIMCAPS CO retrieval results (focus day 2015-02-17)

July 2017 – Montenegro Fire



- The International Charter aims at providing a unified system of space data acquisition and delivery to those affected by natural or man-made disasters through Authorized Users.
- Each agency member has committed resources to support the provisions of the Charter and thus is helping to mitigate the effects of disasters on human life and property.
- https://disasterscharter.org/web/guest/home



July 2017 – Croatia and Montenegro Fires





Left: Smoke and flames rise from a fire in the village of Podstrana, near the Adriatic coastal town of Split, on July 18, 2017. Montenegro asked for international help to fight wildfires on the Lustica peninsula on the country's Adriatic coast, while forest fires in neighboring Croatia spread to suburbs of the coastal city of Split.

Right: NASA image courtesy NASA MODIS Rapid Response Team https://www.nasa.gov/image-feature/goddard/2017/nasa-sees-smoke-from-fires-incroatia-and-montenegro



NUCAPS FSR CO retrieval skills: July 27 2017 – Croatia and Montenegro Fires





Current NUCAPS trace gas JPSS funded initiatives

This is not validation in the traditional sense, it is developing new users applications.

1. Carbon Monoxide and Methane product evaluation (NESDIS/STAR & OAR/ESRL/CSD).

Scope: Models are used to interpolate the sparse aircraft observations to the satellite temporal, spatial, and vertical sampling characteristics for detailed validation. NUCAPS (and AOD from VIIRS) will be used within IDEA (Infusing Satellite Data into Environmental Air Quality Applications)

- I. PI Greg Frost: "Understanding emissions and tropospheric chemistry using NUCAPS and VIIRS"
- II. PI Brad Pierce: "High Resolution Trajectory-Based Smoke Forecasts using VIIRS Aerosol Optical Depth and NUCAPS Carbon Monoxide Retrievals."
- References:
 - Songnex: <u>http://esrl.noaa.gov/csd/projects/songnex/</u>
 - SENEX: http://www.esrl.noaa.gov/csd/projects/senex/
 - IDEA: <u>http://www.star.nesdis.noaa.gov/smcd/spb/aq/</u>

2. Use of NUCAPS Ozone in hurricane extra-tropical transition applications (SPORT)

Scope: Migrate AIRS/SEVIRI product to NUCAPS O₃ with VIIRS RGB. To conduct a product demonstration and assessment with the NHC, WPC and OPC forecasters

- I. PI Emily Berndt: "investigation of NUCAPS T(p), q(p), and O3(p) to study extra-tropical transition of hurricanes"
- Reference:
 - https://nasasport.wordpress.com/2016/10/05/nucaps-soundings-and-hurricane-matthew/



Few lessons learned on users needs in preparation for the next field campaign (FIREX 2018)

- Users need to know spatial and vertical error covariance
 - Many of the signals we see have seasonal or spatial variability in the information content.
 - Trace gas retrievals are sensitive to stratospheric-tropospheric exchange. Broad vertical weighting functions tend to mix stratospheric and upper tropospheric contributions together. Averaging kernels should become an integral part of the operationally distributed products.
 - We are working on submitting a formal user request to have NUCAPS averaging kernels operationally distributed.
- Users need reprocessing capability to study long-term stability of an algorithm.
 - All archived data ("granule" processing)
 - Global "gridded" data sub-sets (for rapid evaluation of algorithm modifications)
 - All validation datasets (including radio-sonde, aircraft match up datasets)
- Users need user-friendly data formats (netcdf4 is generally preferred)
- Users need more sophisticated QCs than what is used in current operations
 - Original QC was developed to demonstrate that we meet requirements
 - Some "green" scenes are bad, some "red" scenes are good
 - We need to develop QCs specifically tailored for trace gas applications
- Users need near real time access to NUCAPS high resolution operational products (essential for applications involving fire trajectories and air quality).
 - FSR NUCAPS soon to be installed in the NOAA DB.
 - This is in preparation of the future NOAA FIREX 2018 campaign (http://www.esrl.noaa.gov/csd/projects/firex/).

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Future upgrades and conclusions remarks

Coming next

- We are working on a formal request for a NUCAPS NH₃ product.
- What defines the need for a trace gas operational product?
 - Just because we can retrieve a product, it does not mean that we should do it.
 - We need a real time, vetted, institutional user: EPA, National Forest Service, DOA, etc.
 - We need users that need archived consistent products: NUCAPS CO2 might serve as forecast climatology for the National Weather Service.

Conclusion remarks

- We would like to support any project supported by the NOAA AC4 Program to engage new potential users and gain insights on the applicability of our products.
 This will ultimately lead to a <u>user requirement</u> to justify the effort of
 - maintaining and improving current and
 - developing new

trace gas operational products.





NUCAPS Retrieval Algorithm Flow Chart



- I. A microwave retrieval module which computes Temperature, water vapor and cloud liquid water (Rosenkranz, 2000)
- II. A fast eigenvector regression retrieval that is trained against ECMWF and all sky radiances which computes temperature and water vapor (Goldberg et al., 2003)
- III. A cloud clearing module (Chahine, 1974)
- IV. A second fast eigenvector regression retrieval that is trained against ECMWF analysis and cloud cleared radiances
- V. The final infrared physical retrieval based on a regularized iterated least square minimization: temperature, water vapor, trace gases (O3, CO, CH4, CO2, SO2, HNO3, N2O) (Susskind, Barnet, Blaisdell, 2003)



Definition of "Spectral Purity"



The finite spectral resolution of the instrument does not allow for *spectral purity*. Specifically, in the infrared domain, the signal associated with a given channel of nominal frequency v is, in reality, the result of multiple molecular rotovibrational transitions whose spectral range of occurrence falls in within the spectral resolution Δv of the channel.

NUCAPS: a sequential, iterated, linearized, weighted, regularized least square fit



$$\Delta R_{n} = K_{n,L}^{i} \Delta X_{n,L}^{i} + \mathcal{E}_{n}$$
$$\mathcal{E}_{n} = NEDT_{n} + \delta R_{CCR} + \delta RTA_{n} + \sum K^{j} \delta X^{j}$$
$$X_{L} = X_{L}^{a} + \left[K_{L,n}^{T} \cdot S_{\epsilon n,n}^{-1} \cdot K_{n,L} + S_{aL,L}^{-1}\right]^{-1} \cdot K_{L,n}^{T} \cdot S_{\epsilon n,n}^{-1} \cdot (R_{n} - K_{n,L} \cdot X_{L}^{a}) \pm \delta X$$



NUCAPS FSR CO DOFs

||H||9 180 150 120 150 180 90 NoData QC fail 0.0 0.2 0.4 0.6 0.8 1.0 1.2 NOAANESDIS/STAL

NUCAPS IR/MW Carbon Monoxide Degrees of Freedom Des (v1.5) 17 Feb 2015









Status of NUCAPS Full Spectral-Resolution Trace Gas EDR Validation

Nicholas R. Nalli^{1,2}, A. Gambacorta^{3,2}, C. Tan^{1,2}, F. Iturbide-Sanchez^{1,2}, C. D. Barnet³, X. Xiong^{1,2}, M. Wilson^{1,2}, K. Zhang^{1,2}, *et al.*

¹IMSG, Rockville, Maryland, USA ²NOAA/NESDIS/STAR, College Park, Maryland, USA ³STC, Columbia, Maryland, USA

> 2017 STAR JPSS Annual Meeting College Park, Maryland, USA August 2017



• SNPP Sounder Trace Gas EDR Validation Truth Dataset collection

- Ozone
 - NOAA AEROSE: V. R. Morris, E. Joseph, M. Oyola (HU/NCAS); D. Wolfe (NOAA/ESRL); NOAA PIRATA Northeast Extension (PNE); NOAA Educational Partnership Program (EPP) grant NA17AE1625, NOAA grant NA17AE1623
 - CalWater/ACAPEX: R. Spackman (STC); R. Leung (PNNL); C. Fairall, J. Intrieri (NOAA); N. Hickmon, M. Ritsche, A. Haruta, and the ARM Mobile Facility 2 (AMF2)
 - World Ozone and Ultraviolet Radiation Data Centre (WOUDC) data contributors (DWD-GRUAN, & INPE, & KNMI, & NASA-WFF, & SMNA. <u>http://www.woudc.org</u>
 - SHADOZ: Southern Hemisphere Additional Ozonesondes (A. Thompson et al.)
- Carbon Trace Gases
 - NASA Sounder Science Team: E. Olsen, T. Pagano, E. Fetzer (NASA/JPL)
 - Total Carbon Column Observing Network (TCCON) (*D. Wunch* et al.) data were obtained from the TCCON Data Archive, hosted by the Carbon Dioxide Information Analysis Center (CDIAC), tccon.onrl.gov
- The NOAA Joint Polar Satellite System (JPSS-STAR) Office (*M. D. Goldberg, L. Zhou, et al.*) and the NOAA/STAR Satellite Meteorology and Climatology Division.
- **STAR soundings team**: *A.K. Sharma, Q. Liu, T. King, W. W. Wolf* (STAR)

Outline



- JPSS Sounder Trace Gas EDR Cal/Val Overview
 - JPSS Level 1 Requirements
 - Validation Hierarchy recap
 - NUCAPS Algorithm
 - v1.5, nominal spectralresolution (NSR) CrIS
 - v2.0 Phase 4, full spectralresolution (FSR) CrIS

NUCAPS IR Ozone Profile EDR Product Evaluation

- v1.5 NSR Review
 - Global ozonesonde ensemble
- v2.0 FSR (Phase 4) Status
 - Global Focus Day ECMWF

- NUCAPS Carbon Trace Gas EDR Product Evaluation (Preliminary)
 - Truth Datasets and Methodology
 - AIRS Version 6
 - TCCON
 - v2.0 FSR (Phase 4) Status
 - Carbon Monoxide (CO)
 - Methane (CH₄)
 - Carbon Dioxide (CO₂)




Status of NUCAPS FSR Trace Gas EDR Validation

JPSS SOUNDER TRACE GAS EDR CAL/VAL OVERVIEW



CrIS Infrared Trace Gases Specification Performance Requirements							
PARAMETER	THRESHOLD	OBJECTIVE					
O ₃ (Ozone) Profile Precision, 4–260 hPa (6 statistic layers)	20%	10%					
O ₃ (Ozone) Profile Precision, 260 hPa to sfc (1 statistic layer)	20%	10%					
O ₃ (Ozone) Profile Accuracy, 4–260 hPa (6 statistic layers)	±10%	±5%					
O ₃ (Ozone) Profile Accuracy, 260 hPa to sfc (1 statistic layer)	±10%	±5%					
O ₃ (Ozone) Profile Uncertainty, 4–260 hPa (6 statistic layers)	25%	15%					
O_3 (Ozone) Profile Uncertainty, 260 hPa to sfc (1 statistic layer)	25%	15%					
CO (Carbon Monoxide) Total Column Precision	35%, or full res mode 15%	3%					
CO (Carbon Monoxide) Total Column Accuracy	±25%, or full res mode ±5%	±5%					
CO ₂ (Carbon Dioxide) Total Column Precision	0.5% (2 ppmv)	1.05 to 1.4 ppmv					
CO ₂ (Carbon Dioxide) Total Column Accuracy	±1% (4 ppmv)	NS					
CH4 (Methane) Total Column Precision	1% (≈20 ppbv)	NS					
CH4 (Methane) Total Column Accuracy	±4% (≈80 ppmv)	NS					

Source: (L1RD, 2014, pp. 45-49)

Validation Methodology Hierarchies



$T/H_2O/O_3$ Profiles

(e.g., Nalli et al., JGR Special Section, 2013)

1. Numerical Model (e.g., ECMWF, NCEP/GFS) Global *Comparisons*

- Large, truly global samples acquired from Focus Days
- Useful for sanity checks, bias tuning and regression
- Limitation: Not independent truth data
- 2. Satellite Sounder EDR (e.g., AIRS, ATOVS, COSMIC) Intercomparisons
 - Global samples acquired from Focus Days (e.g., AIRS)
 - Limitation: Similar error characteristics

3. Conventional PTU/O3 Sonde Matchup Assessments

- WMO/GTS operational sondes or O3-sonde network (e.g., SHADOZ)
- Representation of global zones, long-term monitoring
- Large samples after a couple months (e.g., *Divakarla et al.*, 2006; *Reale et al.* 2012)
- Limitations: Skewed distributions; mismatch errors; non-uniform radiosondes, assimilated into NWP

4. Dedicated/Reference PTU/O3 Sonde Matchup Assessments

- Dedicated for the purpose of satellite validation
- Reference sondes: CFH, **GRUAN** corrected RS92/RS41
- E.g., ARM sites (e.g., Tobin et al., 2006), AEROSE,
 CalWater/ACAPEX, BCCSO, PMRF
- Limitation: Small sample sizes, geographic coverage
- 5. Intensive Field Campaign *Dissections*
 - Include dedicated sondes, some not assimilated into NWP models
 - Include ancillary datasets, ideally funded aircraft campaign(s)
 - E.g., SNAP, SNPP, AEROSE, CalWater, JAIVEX, AWEX-G, EAQUATE

Carbon Trace Gases

1. Numerical Model Global *Comparisons*

- Examples: ECMWF, NCEP/GFS
- Large, truly global samples acquired from Focus Days
- Limitation: Not independent truth data

2. Satellite Sounder EDR Intercomparisons

- Examples: AIRS, OCO-2, MLS
- Global samples acquired from Focus Days (e.g., AIRS)
- Limitation: Similar error characteristics

3. Surface-Based Spectrometer Network Matchup Assessments

- Total Carbon Column Observing Network (TCCON)
- Provide routine independent measurements representing global zones akin to RAOBs
- Limitations: Small sample sizes, uncertainties in conversions to column abundances, different sensitivity to atmospheric layers

4. Intensive Field Campaign *In Situ* Data *Assessments*

- Include ancillary datasets, ideally funded aircraft campaign(s)
- E.g., ATom, FIREX, HIPPO

NOAA Unique Combined Atmospheric Processing System (NUCAPS) Algorithm (1/2)



Operational algorithm

- NOAA Enterprise Algorithm for CrIS/IASI/AIRS (Susskind, Barnet and Blaisdell, IEEE 2003; Gambacorta et al., 2014)
- Global non-precipitating conditions
- Atmospheric Vertical Temperature, Moisture Profiles (AVTP, AVMP)
- Trace gas profiles (O₃, CO, CO₂, CH₄)

• Users

- Weather Forecast Offices (AWIPS)
 - Nowcasting / severe weather
 - Alaska (cold core)
- NOAA/CPC (OLR)
- NOAA/ARL (IR ozone, trace gases)
- NOAA TOAST ozone product
- Basic and applied science research (e.g., *Pagano et al.*, 2014)
 - Via NOAA Data Centers (e.g., CLASS)
 - Atmospheric chemistry research
 - Universities, peer-reviewed pubs

NUCAPS IR O₃

NUCAPS CO



NUCAPS CO₂

NUCAPS Carbon Dioxide at 500mb Asc (v1.8.1HR) 17 Feb 2015



NUCAPS CH₄

NUCAPS Methane at 500mb Asc (v1.8.1HR) 17 Feb 2015





NUCAPS Offline Code Versioning

- Version 1.5
 - Operational system beginning in September 2013
 - Runs on CrIS nominal spectral-resolution (NSR) data
 - Validated Maturity for IR Ozone Profile EDR attained Oct 2016
 - Carbon trace gas EDR validation was not required
- Versions 1.8.x to 1.9.x
 - Preliminary offline experimental algorithms in preparation for CrIS full spectral-resolution (FSR) data
 - Ad hoc CrIS full-resolution radiative transfer algorithm (RTA) and bias correction coefficients
- Version 2.0 (Phase 4)
 - Uses UMBC CrIS full-res (FSR) RTA (L. Strow et al.)
 - Includes IR-only version (risk-mitigation for ATMS loss)
 - Phase 4 Algorithm Readiness Review (ARR) delivered on 6 July 2017
 - Draft ATBD delivered August 2017
 - Code currently being delivered and transitioned into operations





Status of NUCAPS FSR Trace Gas EDR Validation

IR OZONE PROFILE EDR

Science Application: Ozone Hole Over Antarctica





Nalli et al. – 2017 JPSS Annual

NUCAPS IR Ozone and AVTP Zonal Means



NUCAPS v1.5 - Focus Day 17-Feb-2015 Zonal Means

ND ATMOSA

NUCAPS IR Ozone Profile EDR Validation

From Nalli et al.

(2017b)

NSR (v1.5) In Situ Truth Datasets



Collocated Ozonesondes for **O**₃ **Profile EDR**

- Dedicated Ozonesondes
 - NOAA AEROSE (Nalli et al. 2011)
 - CalWater/ACAPEX 2015

Sites of Opportunity

- SHADOZ (Thompson et al. 2007)
 - Costa Rica
 - Hanoi
 - Irene
 - Java
 - Natal
 - Paramaribo
 - Reunion
 - American Samoa
- WOUDC
 - STN043
 - STN053
 - STN107
 - STN101



180[°]W 120[°]W 60[°]W

Geographic Sample Histogram (Equal Area)

FOR Collocation Criteria: $\delta x \le 125 \text{ km}, -240 < \delta t < +120 \text{ min}$



Aug 2017

Nalli et al. – 2017 JPSS Annual

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NUCAPS IR Ozone Profile Coarse-Layer Statistics NSR (v1.5) versus Global Ozonesondes



Retrieval and A Priori



NUCAPS IR Ozone Profile Coarse-Layer Statistics NSR (v1.5) versus Global Ozonesondes



Retrieval and **ECMWF**







NUCAPS FSR Ozone Versus ECMWF





Status of NUCAPS FSR Trace Gas EDR Validation

CARBON TRACE GAS EDR

Science Application: Elevated CO From European Fires, 27 July 2017





Nalli et al. – 2017 JPSS Annual

- **Carbon trace gas EDR validation** versus JPSS program established uncertainty specifications is a **new sounder validation requirement** that began during the transition period to the FSR CrIS NUCAPS
- In response to these new requirements, a validation strategy was devised with preliminary validation of NUCAPS carbon trace gas EDRs conducted leveraging global truth datasets, including
 - ECMWF from Global Focus Days (Cal/Val Method #1)
 - Satellite EDRs from Global Focus Days (Cal/Val Method #2)
 - Aqua AIRS v6
 - Ideally suited given same orbit, retrieves the same constituents as NUCAPS, including total column CO and CH₄; offline v6 runs for CO₂ were made available courtesy of Ed Olsen
 - OCO-2, MLS (future plans)
 - Of high value for inter-satellite stability
 - Total Carbon Column Observing Network (TCCON) (Wunch et al. 2011) Cal/Val Method #3
 - Global network of ground-based FTS that accurately measure total column abundances of CO₂, CO, CH₄, N₂O trace gases
 - Provides "spot checks" for verifying NUCAPS and AIRS
- Collocation Methodology
 - 2-D linearly interpolated FOR used for AIRS versus NUCAPS
 - "VALAR method" used for NUCAPS/AIRS versus TCCON
 - Include all FOR within threshold radius (150 km for 1 Focus Day; 100 km for 2 Focus Days); time window (±6 hours) versus mean TCCON
 - Quality assurance (QA)
 - NUCAPS IR+MW quality flag and AIRS trace gas quality flags
 - NUCAPS trace gas QA flags have not yet been developed, but possible criteria include DoF, Chi-Square and EDR thresholds

- For NUCAPS CO₂, stats are performed simply for atmospheric column averages (in PPMV)
- For NUCAPS CO, CH₄, profile EDRs on 100 RTA layers are integrated to obtain total column abundances (molecules/cm2) (e.g., *Nalli et al.* 2013)

$$\Sigma_x(z) \equiv \int_{z_t}^z N_x(z') \,\mathrm{d}z'$$

$$\implies \Sigma_x(z_s) \approx \mathcal{F}_{\mathrm{BL}} \overline{N}_{x,L_b} \,\delta z_{L_b} + \sum_L^{L_b-1} \overline{N}_{x,L} \,\delta z_L$$

• **TCCON CO, CH**₄ (in dry mole fractions, ppm) are converted to total column abundance Σ_i (molecules/cm²) using the following formula

$$\Sigma_i(z_s) = x_i \left[\frac{N_A p_s}{g M_{dry}} - \varepsilon \Sigma_w(z_s) \right]$$

where x_i is the TCCON-measured dry mole fraction for species *i*, and Σ_w is the H₂O column abundance (provided by NUCAPS retrieval).

• A more rigorous methodology employing the **TCCON averaging kernels** is currently being researched and will be the subject of near-future work



Total Column Carbon Monoxide (CO) EDRs







Nalli et al. – 2017 JPSS Annual

NUCAPS v2.0.5.4 CO – AIRS v6 CO

REDIS CONTRACTOR CONTRACTOR

17 Feb 2015 Focus Day, Accepted Cases





Total Column Methane (CH₄) EDRs 17 Feb 2015 Focus Day, All Cases





Nalli et al. – 2017 JPSS Annual

NUCAPS v2.0.5.4 CH_4 – AIRS v6 CH_4



17 Feb 2015 Focus Day, Accepted Cases





Total Column Carbon Dioxide (CH₂) EDRs 17 Feb 2015 Focus Day, All Cases





NUCAPS v2.0.5.4 CO_2 – AIRS v6 CO_2



17 Feb 2015 Focus Day, Accepted Cases



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Total Carbon Column Observing Network (TCCON) 17 Feb 2015 Focus Day





TCCON (Wunch et al. 2011)

Aug 2017

Nalli et al. – 2017 JPSS Annual

NUCAPS-AIRS vs TCCON Box Plots 17 Feb 2015 Focus Day





NUCAPS v2.0.5.4 acc (17-Feb-15)

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NUCAPS-AIRS vs TCCON Box Plots 17 Feb 2015 Focus Day





NUCAPS v2.0.5.4 acc (17-Feb-15)

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NUCAPS-AIRS vs TCCON Histograms 17 Feb 2015 Focus Day





NUCAPS v2.0.5.4 acc (17-Feb-15)

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Total Carbon Column Observing Network (TCCON) 17 Feb 2015 and 17 Jul 2015 Focus Days





TCCON (Wunch et al. 2011)

NUCAPS vs TCCON Boxplots 17 Feb 2015 and 17 Jul 2015 Focus Days





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NUCAPS vs TCCON Boxplots 17 Feb 2015 and 17 Jul 2015 Focus Days



NUCAPS v2.0.5.4 acc (17-Feb-15 17-Jul-15)



NUCAPS vs TCCON Scatterplots 17 Feb 2015 and 17 Jul 2015 Focus Days





NUCAPS v2.0.5.4 acc (17-Feb-15 17-Jul-15)

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NUCAPS vs TCCON Scatterplots 17 Feb 2015 and 17 Jul 2015 Focus Days





NUCAPS v2.0.5.4 acc (17-Feb-15 17-Jul-15)

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NUCAPS vs TCCON Histograms 17 Feb 2015 and 17 Jul 2015 Focus Days





NUCAPS v2.0.5.4 acc (17-Feb-15 17-Jul-15)

NUCAPS vs TCCON Histograms 17 Feb 2015 and 17 Jul 2015 Focus Days





NUCAPS v2.0.5.4 acc (17-Feb-15 17-Jul-15)

Aug 2017

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	TCCON Baseline One Focus Day <i>N</i> = 151			TCCON Baseline Two Focus Days <i>N</i> = 128			AIRS Baseline One Focus Day <i>N</i> = <i>O</i> (100,000)			
Trace Gas EDR	BIAS (%)	STD (%)	RMS (%)	BIAS (%)	STD (%)	RMS (%)	BIAS (%)	STD (%)	RMS (%)	
СО	+2.1 (±5.0)	12.9 (15.0)	13.1	+6.0 (±5.0)	8.0 (15.0)	10.0	+3.0 +3.3 (±5.0)	9.2 8.9 (15.0)	9.7 9.5	
CO ₂	-0.3 (±1.0)	0.6 (0.5)	0.7	+0.5 (±1.0)	0.6 (0.5)	0.8	+0.2 +0.1 (±1.0)	0.9 1.0 (0.5)	0.9 1.0	
CH ₄	-3.0 (±4.0)	4.4 (1.0)	5.3	-1.1 (±4.0)	2.6 (1.0)	2.9	+0.6 +0.8 (±4.0)	1.7 1.6 (1.0)	1.8 1.8	
	Yield = 83.4%				Yield = 83.7%			Yield = 83.4%		



	TCCON Baseline One Focus Day <i>N</i> = 151			TCCON Baseline Two Focus Days Outlier Sites Removed			AIRS Baseline One Focus Day <i>N</i> = <i>O</i> (100,000)		
Trace Gas EDR	BIAS (%)	STD (%)	RMS (%)	BIAS (%)	STD (%)	RMS (%)	BIAS (%)	STD (%)	RMS (%)
СО	+2.1 (±5.0)	12.9 (15.0)	13.1	+4.7 (±5.0)	7.1 (15.0)	8.5	+3.0 +3.3 (±5.0)	9.2 8.9 (15.0)	9.7 9.5
CO ₂	-0.3 (±1.0)	0.6 (0.5)	0.7	+0.5 (±1.0)	0.5 (0.5)	0.7	+0.2 +0.1 (±1.0)	0.9 1.0 (0.5)	0.9 1.0
CH ₄	-3.0 (±4.0)	4.4 (1.0)	5.3	-0.6 (±4.0)	1.8 (1.0)	1.9	+0.6 +0.8 (±4.0)	1.7 1.6 (1.0)	1.8 1.8
	Yield = 83,4%			Yield = 83.7%			Yield = 83.4%		

NUCAPS EDR Maturity Status



	S-NPP EDR Validated Maturity Oct. 2016-Current: NUCAPS							
	Sensor	Product	Priority	Validated Maturity Review Date & Status		Review Panel Recommendations		
Slide courtesy of Lihang Zhou, STAR/JPSS	CrIS/ATMS	Atm. Vertical Moisture Profile (AVMP)	3	*	√ v	September 2014		
	CrIS/ATMS	Atm. Vertical Temperature Profile (AVTP)	3	*	√ v	September 2014		
	CrIS/ATMS	Ozone Profile EDR	3	Oct-2016	√ v	Panel recommended the following: (1) Work with EMC and NWS on user applications (2) Validate against OMPS NP data (3) Extend validation to more ozonesondes		
	CrIS	Outgoing Longwave Radiation	3	Oct-2016	√ v	Panel recommended the following: (1) Investigate the use of VIIRS for helping to understand the differences between OLR from CrIS and CERES. (2) Compare anomaly events from CERES OLR (e.g. ENSO, MJO) to CrIS OLR data (3) Provide information about how algorithm will be updated to utilize CrIS FS data		
	CrIS/ATMS	Carbon Monoxide	4	&	🗸 Р	Validated Maturity Review for Fall 2017		
	CrIS/ATMS	Carbon Dioxide	4	&	🗸 Р	Validated Maturity Review for Fall 2017		
	CrIS/ATMS	Methane	4	&	🗸 Р	Validated Maturity Review for Fall 2017		

*Product reached validated maturity in September 2014.

[&]Product reached provisional maturity in January 2013. NUCAPS Phase IV/Part II ARR completed on July 6, 2017.



O₃, CO, CH₄, CO₂ Trace Gas Summary



- NUCAPS IR ozone (O₃) profile EDR products generally meet JPSS Level 1 requirements
 - NUCAPS (v1.5 NSR) reached Validated Maturity based upon coarse/broad layer statistical analyses versus
 - Collocated global ozonesondes, including dedicated ozonesondes (Validation Hierarchy Method #4)
 - Global Focus Day (17 February 2015) ECMWF output (Validation Hierarchy Method #1)
 - Statistics are comparable to those reported by *Divakarla et al.* (2008) for the AIRS Version 5 ozone product
 - NUCAPS Phase 4 v2.0 FSR also meets Level 1 requirements and have reached Provisional Maturity based upon coarse/broad layer statistical analyses versus global Focus Day ECMWF
 - Statistics are comparable to the ozonesonde-validated NUCAPS v1.5
- **Carbon trace gas EDR validation** versus program-established uncertainty specifications was a new task beginning with the transition to the FSR CrIS NUCAPS. Preliminary validation versus AIRS and TCCON truth datasets show the products are reasonably close to meeting JPSS Level 1 requirements

• Next Steps / Future Work

- Acquire additional Focus Days to increase the TCCON data sample
 - Currently collecting 2 additional days for Spring and Autumn seasons
- Apply TCCON AKs
- Develop objective methods for eliminating TCCON "outlier sites"
 - Check for altitude gradients within collocation radii
 - Check for land/sea boundaries within collocation radii
- Develop Trace Gas EDR quality flags
- Acquire field campaign datasets (e.g., ATom)
- Further optimization of NUCAPS trace gas *a priori* (viz., O₃, CH₄ and CO₂)




Status of NUCAPS FSR Trace Gas EDR Validation

THANK YOU! QUESTIONS?

FORWARD MODEL IMPROVEMENTS: PRESENT AND FUTURE

L. Larrabee Strow, Sergio deSouza-Machado, Steven Buczkowski JPSS STM – August 14, 2017

Joint Center for Earth Systems Technology and UMBC Department of Physics

Outline

- CrIS FSR forward model
- CrIS minor gas trend retrievals
- Single footprint retrievals

FSR Forward Model

Summary of FSR SARTA

- CrIS high-resolution ILS
- HITRAN 2012 (vs 2008 in original CrIS RTA)
- LBLRTM Line Mixing for CO2 and CH4, H2O continuum
- UMBC line-by-line for water
- Code Change: improved reflected thermal for high secant angles
- Tested on 750+ profiles (from ECMWF selected subset), regressed on 49 profiles
- Error covariance estimates available from 750+ profile testing

kCARTA (LBL) partially trained on LBLRTM allows us to compute 25,000 plus monochromatic test profiles!

Parameterization Errors



Some increase in Mean/Std errors with SAF. Can diagonose with so many test cases.

Bias/Std versus ECMWF: 3 days ocean clear



Wavenumber (cm -1)

Secant Angle Dependence



- Fit for slope of each channel versus secant of viewing angle
- Used 10 angles from nadir to max scan angle
- Errors are about ±0.1K except less near 700-720 cm⁻¹

RTA (SARTA) Parameterization Error Correlations

Raw: No Noise



- 705 global profiles
- Computed correlations for LBL (kCARTA) minus fast RTA (SARTA)
- Same kCARTA used to create SARTA parameterizations

Water region errors (no shown) highly correlated.

Future Improvements?

- Testing neural-net (2-3 layer, feed-forward) for parameterization of absorption coefficients
- Done for each optran layer, but hoping can use one net for all layers
- Using SAF 705*7 profile set, can expand to 25,000 profiles
- Really helps finding problem profiles, regression set is pretty good!



Neural net error for 1691.25 cm⁻¹ channel versus total column water

CrIS Minor Gas Trends

OE Minor Gas Retrievals from BT Trends: CO₂



MLO: 2.49 ppm/year (last 5 years) CriS Tropics: 2.56 ppm/year (last 5 years) Difference = 0.0035K/year in possible drift!

OE Minor Gas Retrievals from BT Trends: CH₄:



SST vs ERA (ghrsst): 0.0035K/year in BT units CH₄ vs MLO: ~0.01K/year (MLO: 8.6 ppb/year, CrIS: 8.1 ppb/year)

CrIS All-Sky Trends



Latitude variability high: $\pm 0.2\text{-}0.3\text{K/year}$ BUT within 2σ estimated uncertainties.

This is a short time period. 14-year AIRS trend is ${\sim}0.015K \pm 0.01K.$

Single Footprint Retrievals with SARTA

Scattering SARTA

- Designed to mimic what *can be retrieved*.
- Very simple scattering, 2X slower than clear SARTA
- Two scattering layers, some mix of ice cloud, water cloud, aerosol (dust, volcanic ash)
- Two major liens vs PCRTM tests with ECMWF (Xu Liu)
 - 2 layers, no statistical cloud overlap computations
 - Less accurate scattering, likely only an issue with solar in SW

Single Footprint Retrievals

- Cloud initialization by using NWP model (ERA) clouds (find close-by grid point similar to observations)
- Could be initialized with climatology
- Fixed cloud heights, fit for cloud amount and particle size
- Tested first with smooth a-priroi climatology
- Then, move to ERA a-apriori
- Mostly used for trend retrievals. Hope to use for radiosonde intercomparisons
- Lots of testing, mostly analyzing special cases.

OE framework very good at accuracy estimates, let's you naturally Q/A cloud problems (thick clouds)

ECMWF 91 to SARTA 2 layer cloud conversion



Comparison to PCRTM (with Statistical Cloud Overlap)



Global Simulation from ERA



Retrieval Sample: RH for Atmospheric River



Cirrus Cloud Optical Depth Comparisons with AIRS



Cloud Top Height Comparisons with MODIS



What are NUCAPS trace gas products good for?

Nadia Smith* In collaboration with JPSS NUCAPS team and PGRR initiatives

(addressing the white elephant in the room)



O_3 CH_4 N_2O CO HNO_3 CO_2 SO_2

Who uses NUCAPS trace gas products operationally?

Do you know anyone who makes (or has made) a real-world decision with information provided by NUCAPS trace gas products?

(...crickets...)

Why not?

What are the NUCAPS trace gas products?

By-products of physical retrieval system:

(1) ...to stabilize T/q retrievals

CH

(2) ... to enable full connectivity between EDR + SDR for quality monitoring

HNO

CO.

(3) ... to enable air chemistry applications from weather satellite systems

(CO)

What is the baseline? Where are we at, exactly?

(1) NUCAPS trace gas <u>validation</u> (NOAA/STAR)

– Operational requirements

(2) NUCAPS trace gas evaluation (NOAA/JPSS PGRR initiatives)

- Suitability for real-world applications

Creative exploration in strong, productive, multi-agency partnerships
(NOAA/ESRL, NOAA/STAR, UW/SSEC; CSPP; STC, etc.)

NOAA PGRR – Sounding and Fire+Smoke Initiatives

JPSS Proving Ground/Risk Reduction (PGRR) project is a collaborative effort combining expertise in satellite retrieval development (STC), airborne trace gas measurements (ESRL/CIRES), and satellite trace gas validation (STAR/CIMSS) to characterize NUCAPS retrieval quality, with the goal of improving the accuracy of the NUCAPS daily global measurements of methane (CH4) and carbon monoxide (CO).

2014 NOAA CrIS Atmospheric Chemistry Data User's Workshop Report

(http://docs.lib.noaa.gov/noaa_documents/OAR/CPO/AC4/CrIS_workshop_2014.pdf) which concluded "that the current state of validation of the NUCAPS trace gas retrievals is insufficient for the use of these retrievals in most atmospheric chemistry applications" and recommended that 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".



Comparisons between RAQMS and in situ CO measurements during SONGNEX show that RAQMS has a mean high bias of 29ppbv above 700mb and tends to overestimate the observed mid tropospheric variability

Brad Pierce (NOAA/STAR); Greg Frost (NOAA/ESRL)

NOAA P-3 aircraft flight paths over the western US during the **SONGNEX field campaign**, March-April, **2015**.



NUCAPS (FSR CrIS)

RAQMS

Comparisons between bias corrected RAQMS and NUCAPS mid tropospheric CO suggests that NUCAPS has a 6.8 ppbv high bias relative to the in situ aircraft measurements

In **2016** CSPP NUCAPS supported a field campaign in real-time (ENRR) for the first time.

Building on lessons learned, CSPP NUCAPS will support FIREX in 2018/2019

Brad Pierce (NOAA/STAR)



CSPP NUCAPS in IMAPP application

http://cimss.ssec.wisc.edu/idea-i/USozone/

Real-time stratospheric intrusion forecasts

The background basemap is the daily AIRS, IASI, or CrIS Dual Regression (CSPP HSRTV) Ozone retrievals at 516mb, which is used in conjunction with Dual Regression dewpoint temperature retrievals to initialize trajectories which show where the stratospheric intrusion (high ozone/dry air) is expected to move in the next ~48 hours. The products are derived from AIRS, IASI and CrIS data acquired and processed directly from the Terra, METEOP-A, and SNPP satellites, respectively

As soon as CrIS FSR SDR is available in CSPP we will ingest NUCAPS CO retrieval in IDEA-I to initialize smoke dispersion forecasts

Brad Pierce (NOAA/STAR)



User-Developer partnership helps evaluate FSR NUCAPS CO ahead of operational deployment

Ft. McMurray Fire; 1-16 May 2016: NUCAPS CO vs RAQMS

FSR NUCAPS with MOZART FG

RAQMS CO MR @ 500 hPa

RAQMS CO at 500 hPa 20160502 06Z

FSR NUCAPS with MOPITT FG

NUCAPS CO with MOZART FG at 500 hPa 20160502 AM orbit







Brad Pierce 6 April 2017: "Since we have aircraft measurements in the SH with ATom, it might be interesting to compare all three first guess retrievals during the Atom flights."







Brad Pierce (NOAA/STAR)



Brad Pierce

The Real-time Air **Quality Modeling** System (RAQMS) aerosol analysis captures the timing and magnitude of the surface smoke over the Pacific Northwest during the July 25-August 8, 2017 period.

Comparisons between RAQMS and NUCAPS CO columns can be used to evaluate the NUCAPS CO retrieval





Brad Pierce (NOAA/STAR)

RAQMS vs FSR NUCAPS Mid-Tropospheric CO

RAQMS vs NUCAPS mid-trop CO; Night time RAQMS vs NUCAPS mid-trop CO; Day time RAQMS vs FSR NUCAPS AM Mid-Tropospheric (700-200mb) CO July 30-August 07, 2017 RAQMS vs FSR NUCAPS PM Mid-Tropospheric (700-200mb) CO July 30-August 07, 2017 r= 0.396380 0.49221(vqdd) 00 (8 S **Cloud artifacts** 120 100 140 100 120 140 NUCAPS CO (ppbv) NUCAPS CO (ppbv) 20 100 40 60 80 20 Counts Counts
NUCAPS CO₂ helps determine T/q retrieval quality

Comparing NUCAPS Temperature with NUCAPS CO₂ highlight cloud contamination not filtered out by QC

Temperature @ 850 hPa



Column integrated CO2



User-Developer partnership helps evaluate NUCAPS CO applications

investigating the presence of elevated H2O mixed layer due to large scale biomass burning

Carbon Monoxide [500hPa]





User-Developer partnership helps evaluate NUCAPS CO applications

Carbon Monoxide [500hPa]

H2O Mixing Ratio [500hPa]



With NUCAPS it is possible to investigate CO emissions as well as the change in moisture regime due to large scale burning

We have done (and continue to do) validation

We have determined that there is potential for strong applications

So what is next?

NUCAPS T/q used in AWIPS to monitor fire weather



NUCAPS Sounding

- A noticeable inversion was detected near/just above 700mb.
- Compared to HRRR, RAP, and NAM soundings taken at a similar time, guidance was unable to detect this feature.
- Decided to investigate a smoke plume seen from KBLX radar



NUCAPS T/q used in AWIPS to monitor fire weather



Slide by Michael Bowlen; HWT 2017

- "The placement of the fire and smoke plume suggests some accuracy of the NUCAPS capture of the inversion, which is missing from model guidance."
- "Additionally, it has been noticed that as convection has pushed eastward this afternoon, it's intensity has been decreasing, which could be an impact of the inversion."

What about NUCAPS trace gas products – would they have been valuable here in AWIPS? shop 🛔

http://www.npr.org/sections/thetwo-way/2017/03/03/518323094/rise-in-smog-

in-western-u-s-is-blamed-on-asias-air-pollution the two-way breaking news from NPR

AMERICA

3

8+

 \sim

Smog In Western U.S. Starts Out As Pollution In Asia, Researchers Say

March 3, 2017 · 10:21 AM ET

BILL CHAPPELL



Nitrogen oxide pollution in India and China is offsetting U.S. gains in cutting emissions, researchers say. This photo from October shows road traffic, along with smoke and smog, in front of the landmark India Gate in New Delhi.

"A <u>global perspective</u> is necessary when designing a strategy to meet US O₃ air quality objectives," the scientists wrote

They concluded that the spike in man-made emissions in Asia "is <u>the major driver</u>" of the rise in ozone levels in the western U.S. for both spring and summer in recent decades.

Lin et al. 2017, ACP, doi.org/10.5194/acp-17-2943-2017

How can this research make its way into the public domain? NUCAPS has the quality and coverage to contribute to air <u>quality monitoring at global scales...</u>

Manish Swarup/AP

"... even quick-look images of CO ... during fire periods would be very useful to us. We don't need a fancy display" Greg Frost (NOAA/ESRL)

"Now-casting tools are important in case of disasters?" Tony Wimmers (SSEC/CIMSS)

"We need to be able to monitor trace gases over time" Monica Kopacs (NOAA/CPO)

<u>https://worldview.earthdata.nasa.gov/</u> <u>https://realearth.ssec.wisc.edu/</u> <u>http://www.esri.com/</u>

We need more options for interactive display Quality Validation -> Application Evaluation -> Every-day Verification

O_3 CH_4 N_2O CO HNO_3 CO_2 SO_2 The questions really should be:

Do you know what NUCAPS trace gas products look like for today?

Will you be able to look at NUCAPS trace gas products tomorrow when this meeting is over?

JOAA • NESDIS JPSS Joint Polar Satellite System



A JPSS Proving Ground/Risk Reduction Project

2017 STAR JPSS Annual Meeting

Evaluating NUCAPS CH_4 and CO

NOAA OAR ESRL: Gregory Frost, S. McKeen, L. Zhang,
R. Ahmadov, W. Angevine, J. Brioude, Y. Cui, K. Froyd,
C. Granier, G. Grell, S.-W. Kim, K. McKain, D. Murphy,
T. Ryerson, J. Roberts, K. Rosenlof, J. Schwarz,
C. Sweeney, M. Trainer, C. Warneke
STC: N. Smith, A. Gambacorta, C. Barnet
NOAA NESDIS STAR: R. B. Pierce
NOAA NESDIS NCEI: C. Elvidge

Close collaboration of ESRL, NESDIS, and STC

- Critical to project's success
- Retrieval developers work directly with science users
- Leads to improved algorithms and products
- Adds value to PGRR investment

NOAA OAR's Atmospheric Composition Tools



Observing the atmosphere at multiple spatial and temporal scales with a suite of complementary approaches

State-of-the-art earth system modeling and data analysis

http://www.esrl.noaa.gov



Approach for this project

Aircraft data from field research studies are the basis of our NUCAPS evaluations, providing...

- high accuracy and precision
- fine horizontal and vertical resolution
- repeated sampling

6/29/13, 16:38-21:46 UTC, Total Precipitable Water (cm)





Atmospheric chemical-transport models evaluated and improved by aircraft data enable direct assessment of NUCAPS trace gases and meteorological products, by...

6/29/13, 16:38-21:46 UTC, mid-trop. CH₄ (ppbv)

- Extending temporal and spatial domain beyond sparse aircraft sampling
- Simulating atmospheric quantities to match NUCAPS retrievals

NUCAPS - Model Comparisons \rightarrow Improved Retrievals



Initial comparisons of NUCAPS data suggested issues with NUCAPS CH₄

 NUCAPS trace gas retrievals used quality control (QC) thresholds optimized for meteorological variables

STC refined its NUCAPS retrieval algorithms

Updated, more restrictive
 QC thresholds specific to
 CH₄ and to 7 other trace
 gases

Assessing NUCAPS Scale Variance

How do we characterize NUCAPS true signals versus noise?

• Assess spatial averaging needed to produce meaningful NUCAPS trace gas data

Decomposition of time series into orthogonal functions has previously been used to analyze the temporal or spatial variance of a measurement

- Dynamic turbulence within the atmosphere is known to be the determining factor in the scale dependence of variance
- Chemical constituents display same scale dependence as thermodynamic and momentum-based quantities (Tuck and Hovde, 1999)
- Use power spectrum analysis of scale variance to determine the quality of NUCAPS retrievals

Time series of aircraft and model CO



Power spectra of aircraft and model CO



Domain for comparisons of NUCAPS to model

NUCAPS total precipitable water

1 June 2013 shown 1 June – 15 July 2013 data were analyzed

Colored pixels = No QC flag filtering **Dotted lines** = 6 NUCAPS tracks that meet QC criteria



Power spectra: NUCAPS and model column CH₄



Power spectra: NUCAPS and model 500-hPa CH₄



Power spectral slopes: NUCAPS, model, aircraft



Spectral Slope (unitless)

Interim conclusions from the project

- Aircraft research observations provide evaluation of atmospheric model
- Evaluated model in turn provides comparison data for NUCAPS retrievals
- Aircraft-model-NUCAPS comparisons → customized trace gas QC thresholds
 - Improved NUCAPS retrievals
 - Larger NUCAPS science dataset compared with operational products
- Scale variance analysis helps distinguish NUCAPS true signals vs. noise
- NUCAPS CH₄ data are meaningful with adequate spatial averaging:
 - *vertically* over full tropospheric column + *horizontally* at scales \geq 200 km
 - *vertically* in mid-troposphere + *horizontally* at scales \geq 340 km
- Need full spectral resolution CrIS radiance products for similar analysis of NUCAPS CO
- In-situ observations should be averaged similarly for meaningful comparison to NUCAPS
 - Averaging limits direct comparison opportunities, thus necessitating use of evaluated chemical-transport models for understanding NUCAPS retrievals

Ongoing work: Atmospheric Tomography Mission



https://espo.nasa.gov/home/atom/content/ATom

NASA's Atmospheric Tomography Mission is conducting continuous pole-topole profiling from 0.2 to 12 km altitude in 4 seasons between 2016 and 2018.

Within NOAA's NGGPS (Next Generation Global Prediction System), ATom data are used to assess performance of global chemical-transport models.

ATom provides excellent evaluation opportunities for JPSS trace gas and aerosol products.

Ŕ

55 2019 NOAA & NASA 500 aircraft studies 450 400 350 45 latitude 35 -P3 aircraft max range 30 for single flight example flight Fires Augu -125 -120-115-110-105

Ongoing Work: Fire Influence on Regional and Global Environments

Experiment (FIREX)

FIREX is NOAA's multi-faceted wildfire research program

- Emissions
- Chemical transformations Model evaluation
- Coordinate with others:



FIRE-Chem FA

n FASMEE

WE-CAN

JPSS fire detection products and trace gas and
 aerosol retrievals will be critical tools for mission
 planning/forecasting and analysis of aircraft data

Next Steps

- Finalize scale variance analysis
- Continue model validation with ATom data
- Analyze NUCAPS CH₄ and CO during ATom deployments
 - Need full spectral resolution CrIS CO data
- Begin planning for FIREX in 2019, and explore applications of JPSS fire-detection and trace gas products



Recent Improvement of NUCAPS CH₄ from CrIS FSR Data

Xiaozhen (Shawn) Xiong^{1,2}, Lihang Zhou² Antonia Gambacorta^{1,3}, Nick Nalli^{1,4}, Changyi Tan^{1,4} Flavio Iturbide-Sanchez^{1,4}, Kexing Zhang^{1,4}

¹CICS-MD ²NOAA/NESDIS/STAR ³ STC Inc ⁴ IMSG

4th NOAA JPSS Meeting, College Park, MD, 2017

1



Outline

Recent Improvements in CH₄ Retrievals from CrIS FSR Data

- Sensitivity (mid-upper troposphere) and Requirement of CH₄ products (based on total amount) --- need a good
 CH₄ firstguess in the lower troposphere;
- Optimization: First guess, Channel Selection, and tuning;
- > Quality control (CH_4QC) to be added soon;

Validation: Comparison of CrIS CH₄ profiles with model, AIRS and TCCON data;

- Examples:
 - Monitoring the leakage of CH₄ from California Aliso Canyon Oil Field and Gas Storage Facility;
 - Monitoring the CO plume from 2016 Fort McMurray wildfire; Monitoring the CO plume from Indonesia Fires (9/20-11/8, 2015);
- Summary and Future works



Requirements of Trace Gases Products from CrIS

	EDR Attribute	со	CO ₂	CH ₄
Under Contraction of the formation of th	Vertical Coverage	Total Column	Total Column	Total Column
	Horizontal Resolution	100 km	100 km	100 km
	Mapping Uncertainty, 3 sigma	25 km	25 km	25 km
CH4, ppb 187 178 183	Measurement Range	0 – 200 ppbv	300 – 500 ppmv	1100 – 2250 ppbv
	Measurement Precision	15%	0.5% (2 ppmv)	1% (~20 ppbv)
	Measurement Accuracy	±5%	±1% (4 ppmv)	±4% (~80 ppbv)
	Refresh	24 h	24 h	24 h

Note



Sensitivity of CrIS to CH₄





•Major sensitivities are in the mid-upper troposphere – not near the surface where the variation is impacted by emissions;

•Sensitivities in the polar are lower than tropics and mid-latitude



CH₄ Total Amount Error

assuming 5% error of CH4 profile in lower troposphere (below 800 hPa)



Assuming 5% error of CH4 profile in lower troposphere(below 800 hPa), the error in total amount is about 1.2%.

- to meet the requirement of total amount in 1%(accuracy) is hard;
- It requires a very good a priori





CH₄ First-guess Update





--- Old fg is the one used in AIRS-V7 and NOAA IASI system



Continued Optimization: Channel Selection (1)



Current one – delivered in July

Updated one – to be delivered in Oct/Nov



Continued Optimization(2): Re-tuning to CH₄ bands



- \succ CH₄ is very sensitive to upstream temperature and water vapor products;
- Cloud-clearing is a good thing to the yield of retrievals but could be poisonous to trace gases products;



- 1) Using SARTA to simulate the global radiance with inputs
 - T,Q profiles from NUCAPS retrievals;
 - CH_4 , N_2O and CO_2 from model simulations;
- 2) read CCR and applied QC (MW+IR) = 0;
- 3) Computed the difference of $[R_{simu} R_{CCR}]_{;}$
- 4) Modified the tuning file in CH₄ bands ONLY (from 1200-1360 cm⁻¹) → no impact to T & q products;

One day data (45°S-45°N) on 2/17/2015 is used;

Comparison of CH₄ from AIRS, IASI and CrIS (20160508, @515hPa) – NO QC to CrIS CH₄ products





ATMOS



1850.0

1750.0

1783.3

1816.7



1883.3

1916.7

IASI-A

1950.0

1950.0



Examples of Quality Control (CH₄QC)



- For two granules
- Left panels: red lines are from current version and black lines are from updated retrievals;
- Right panels: Profiles from new version and after using CH₄QC





1800.0

1825.0

1850.0

Example of CH₄ map with the CH₄QC



1875.0

1900.0

1925.0

1

With CH₄QC

CH4 515.720 20151023



1000 0	1005.0	1050.0	1075.0	1000.0	1005.0	1050.0
1800.0	1823.0	1820.0	1875.0	1900.0	1925.0	1920.0


Yields after using CH₄QC

	Descending	Yield (%)	Percentage relative to NO CH ₄ QC (%)
r	QC=0	37.4	45.0
50.8% 1	QC=1	13.4	16.0
	QC=2	49.2	

54.7% -	Ascending	Yield (%)	Percentage relative to NO CH ₄ QC (%)
	QC=0	43.6	52.0
	QC=1	11.1	13.2
	QC=2	45.2	



Some Results

Validation: comparison with model, AIRS and TCCON data;

Examples:

> Monitoring the leakage of CH_4 from California Aliso

Canyon Oil Field and Gas Storage Facility;

- Monitoring the CO plume from 2016 **Fort McMurray wildfire**;
- Monitoring the CO plume from Indonesia Fires (9/20-11/8, 2015);

Comparison with model CH₄ – improvement is obvious but accuracy is large than 1%

NOAA





Comparison of CrIS and AIRS CH₄



Comparison of CrIS xCO/xCO₂/xCH₄ with TCCON Measurements



MENT



Data of 10 days is used;

 This is a simple comparison by averaging TCCON data within 1 hours of satellite overpass and satellite data within 200 km over the ground site;

Better agreement can be achieved if using of averaging kernels



Example : Largest leakage in U.S. history Aliso Canyon Gas Leakage (10/23/2015- 2/18/2016)



Surface Measurements



Can CrIS Capture the Leakage of CH₄?

ND ATMOSA





Can CrIS Capture the Leakage of CH₄ – cont'd ?

CH4 515.720 20151022



CH4 515.720 20151023



ddd						
1750.0	1783.3	1816.7	1850.0	1883.3	1916.7	1950.0



CH4 515.720 20151024

CH4 515.720 20151023



ppb						
1800.0	1825.0	1850.0	1875.0	1900.0	1925.0	1950.0



Huff and Kondragunta, EOS, V98, 6, 2017

Example of CO: 2016 Fort McMurray Wildfire



MODIS/Aqua captured smoke from the Ft. McMurray wildfire and other Canadian wildfires billowing across the Atlantic Ocean.

CO 515.720 20160508 am



Wildfire Smoke map, 4:30 p.m. May 8, 2016, from Weatherunderground,



Example of CO (2): Fires in Indonesia (9/20-11/8,2015)





Ð

Brownish-gray smoke obscured the island of Borneo from MODIS in October 19, 2015. Image from <u>NASA</u> Earth Observatory.







Summary

- The major sensitivity of CrIS is in the mid-upper troposphere but it is very small in the lower troposphere, so CrIS cannot capture the surface emission.
 5% error of the firstguess in the lower troposphere will lead to 1.2% error in the total amount making it hard to meet the requirement in 1% accuracy.
- 2. Cloud-clearing is a great part from NUCAPS but we have to be very careful to set QC for all trace gases;
- 3. Recent improvements (firstguess, channel selection, tuning and CH_4QC) are promising, but more works need to be done, particularly we need more profile validation using aircraft measurements.
- 4. The examples show some promising results to use CrIS to observe the CO plume from wildfires, and the possibility to capture the CH_4 leakage from Aliso Canyon Oil Field and Gas Storage Facility in California.



Future Works

Trace gases maturity review will be made in Nov/Dec., and this is the deadline for us to finalize the update to trace gases algorithms; Another delivery will be delivered by that time frame;

In addition to the operational system, I will use an offline system with more update to trace gases retrievals to reprocess SNPP CrIS FSR data since Dec.4, 2014 to present. Any update with new sciences can be considered, and these work will help our future update to NUCAPS operational system.







Increase of spectral resolution by 4X in SLW greatly benefits CO retrieval; Not used for CO2 (so far) Increase of spectral resolution by 2X in MLW benefits CH4 retrieval;



CrIS (old) vs AIRS CH₄





Soumi National Polar-orbit partnership (S-NPP) Joint Polar Satellite System (JPSS)



CrIS started to operate in the full spectral resolution (FSR) mode since Dec.4, 2014, with spectral resolution of 0.625 cm⁻¹ for all three bands, thus has 2211 channels as compared to 1305 channels in normal mode;

Using NH₃ Retrievals from the Crosstrack Infrared Sounder to Improve Emission Inventories and Models

M. J. Alvarado¹, K. E. Cady-Pereira¹, M. Shephard², C. R. Lonsdale¹, E. Winijkul¹, C. M. Brodowski¹, D. K. Henze³, and S. Capps^{3,*}

> ¹Atmospheric and Environmental Research ²Environment and Climate Change Canada ³University of Colorado - Boulder *Now At Drexel University



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NH₃ is a PM_{2.5} precursor and reactive N species

$NH_3 + HNO_3 \leftarrow \rightarrow NH_4NO_3$ 2 NH₃ + H₂SO₄ $\rightarrow (NH_4)_2SO_4$

- Increase incidence of cardiovascular and respiratory diseases
- Increase number of CCN
- NH₃ is also one of the most important reactive nitrogen species
 - Leads to soil acidification, water eutrophication (e.g. algal blooms)
 - Ammonia is the least well understood part of the nitrogen cycle



SO₂, NO_X emissions decreasing due to controls, but NH₃ increasing!

Using Satellites to Investigate NH₃ Sources



- TES NH₃ transects over Bakersfield in CalNex suggested a x2 underestimate in afternoon due to diurnal cycle errors (Lonsdale et al., ACP, 2017)
- 2012 CrIS NH₃ is consistent with CalNex TES results.
- Some evidence of a transport error on June 17 – flow along slope not correct?

TES Long-term Megacity Records of NH₃

Mexico City Observations (Cady-Pereira, AMT, 2017)



Why switch to CrIS?

- TES is past its design lifetime and has low spatial coverage
- CrIS could monitor global NH₃ with high spatial coverage for many more years (>2022)



	TES	CrIS
Satellite	AURA	NPP
Available Data	July 2004-present	October 2011-present
Resolution	0.06 cm ⁻¹	0.625 cm ⁻¹
Footprint	5x8 km rectangle	14 km diameter circle
Repeat cycle	Once every 16 days	Daily
Equatorial crossing	1:30 am and 1:30 pm	1:30 am and 1:30 pm
Noise in NH ₃ window	0.09 – 0.12 K	0.03 – 0.06 K





CrIS NH₃ Retrieval: Simulated Spectra



Shephard and Cady-Pereira, AMT, 2015



How CrIS compares with spirals

- January 21, 2013
- Matched each spiral to closest CrIS observation
- 14 spirals were compared
- Used log AK in CrIS operator
- Mismatch between CrIS surface pressure and aircraft surface pressure: shifted aircraft profiles up.





How CrIS compares with spirals

- Same as previous slide for January 30
- Rapidly growing PBL





Atmospheric and Environmental Research

der

NOAA SENEX Campaign (June-July 2013)

NOAA P-3 Aircraft





15.

10.

9.

8.

7.

6.

5.

4.

3.

2.

1.



Feed lot NH₃ emissions overestimated in AL



Environmental Research

CrIS shows other errors in monthly-average NH₃ from CMAQ



- Overestimate of NH₃ in northern AL and GA also in monthly average
- Similar overestimates in NC, MI, VA
- Underestimate along Mississippi River?

aer

CrIS NH₃: N. America Warm Season Average 2013



CrIS NH₃: North America Monthly Averages April to October, 2013



Captures expected temporal and spatial distributions of ammonia

- Spring fertilizer applications (May over Canada)
- Episodic events (e.g. Northern forest fires in middle of summer)

aer

CrIS NH₃: Example of Daily Spatial Variability of Surface NH₃ over North America on August 10 2013

MODIS Infrared: Fire Detection (red) Visible: Cloud (White) Smoke (blue/gray)

100 150 200 250 300 350 800 1100 300 400 500 600 700 900 1000 1200 1300

AQUA MODIS 20130810

CrIS Surface NH, 20130810



CrIS Infrared: NH₃



CrIS NH₃: Fort McMurray forest fires Daily values in May 2016

<u>VIIRS</u>

Infrared: Fire Detection (red) Visible : Cloud (White), Smoke (blue/gray)

<u>CrIS</u> Infrared: Ammonia (NH₃)



Click image to view Movie



Model Evaluation: GEM-MACH Spatiotemporal Emissions

GEM-MACH Emissions

- 15-km emissions from annual/monthly inventory using monthly/weekly/diurnal activity-based temporal profiles
- 20:00UTC hourly snapshot corresponding to satellite overpass
- No forest fire emission included



Model emission improvement study led by Junhua Zhang

CrIS Surface Concentrations

- Monthly Mean
- Satellite overpass (~1:30 local time)
- Includes contributions from forest fire



Sept 2013

Spatial and temporal distributions are generally consistent

- some regions need improvement
 - North Dakota (spring/fall)
- use satellite to improve model spatial and temporal emissions



- CrIS is able to retrieve NH₃ with similar skill to TES, but much higher spatial coverage.
- CrIS NH₃ retrievals compared well with spirals made during DISCOVER-AQ in California.
- CrIS and NOAA P-3 observations show NH₃ emissions from feed lots in northern Alabama are lower than in the 2011 NEI.
- CrIS is able to measure seasonal and spatial patterns of NH₃ from fertilizer applications and fires over US and Canada.
- Ongoing work is being done to use this data to improve NH₃ emission inventories for models.



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- NOAA CSD and SENEX science team (A. Neuman, J. Nowak, J. Holloway, T. Ryerson, A. Middlebrook, J. Jimenez, J. Fry)
- Environment and Climate Change Canada (C. McLinden, M. Shephard)
- EPA (K. Baker, H. Pye)
- UNC CMAS Center (B.H. Baek, Z. Adelman)


Full-chemistry Volcanic Fog Forecast over Hawaii

Daniel Tong, <u>Youhua Tang</u>, Barry Baker, Li Pan, and Pius Lee NOAA Air Resources Laboratory

> Jianping Huang and Jeff McQueen NOAA NWS/NCEP/EMC

Kai Yang Dept. of Atmospheric and Oceanic Science, University of Maryland, College Park

A pulse of magma moving through Kīlauea's east rift zone









(Source: Hawaiian Volcano Observatory: http://hvo.wr.usgs.gov)

Methodology for Modeling Volcanic Emissions



- SO₂ measurement Correlation Spectrometer (COSPEC);
- Simple plume rise:

Distributed from ground to 100 m above;

Plume Rise of Volcanic Emissions

Make it simple since we know so little about it...



- Multiple and moving emitting points;
- Emitting point below surface;
- Dynamic magma movement;
- Difficult to implement plume rise algorithms, such as Briggs (1972).



Kilauea SO₂ Emissions



(Source: Hawaiian Volcano Observatory: http://hvo.wr.usgs.gov)

Model Configurations

Volcano SO2 emissions:

- Summit Emissions: 650 800 tons/day;
- East Rift Zone: ~400 tons/day;
- * Model (National Air Quality Forecast Capability (NAQFC))
 - CMAQ 5.0.2 CB05-AQ-AERO6 gas, aqueous and aerosol chemistry
- * NAQFC's Hawaii Domain
 - > 80 x 52 grid cells (All islands and surrounding water)
- Horizontal resolution: 12x12 km²
- Vertical level: 35 layers
- Meteorological inputs
 - NAM(NMM-B) 12 km
- Lateral boundary conditions
 - GEOS-Chem precursors with Hilo monthly mean ozonesonde



OMPS SO₂ Total Column (DU)

2017-07-11 20:55:00



Model SO₂ Total Column (DU)



(OMPS SO₂ data is downloaded from NASA retrievals, <u>https://so2.gsfc.nasa.gov</u>) ^{8/24/2017} A REAL OF COMPANY OF COMPANY.

OMPS SO₂ Total Column (DU) 2017-07-13 21:58:20





NORR COMPANY

OMPS SO₂ Total Column (DU) 2017-07-14 21:39:15







8/24/2017

Effects on Air Quality







Summary

- With the proper volcano SO₂ emission, we have capability to predict the Hawaii SO₂ plume, which is comparable to the surface measurements.
- OMPS SO₂ retrievals are comparable to the model results. After suitable Cal/Val, it can be used to verify/assimilate Hawaii volcano SO₂ concentration or emission.
- There are still uncertainties in the volcano emissions, such as plume heat fluxes etc, which can be adjusted with the proper satellite retrieval, such as FRP.

Future Works

- 1. Apply the similar OMPS SO₂ product to verify/assimilate the power-plant SO₂ emissions, which is the major SO₂ source over CONUS.
- 2. As SO₂ is the precursor of sulfate, we should be able see PM2.5 and AOT enhancement in the downstream areas, which can be verified with the VIIRS AOT product.

Smithsonian Astrophysical Observatory OMPS Nadir Mapper formaldehyde retrievals



Gonzalo González Abad, Kelly Chance and Xiong Liu STAR JPSS 4th Annual Science Team Meeting 17th August 2017



Outline

• Formaldehyde in the atmosphere

- Smithsonian Astrophysical Observatory OMPS formaldehyde retrieval:
 - Spectral fitting
 - Air mass factor correction
 - Reference sector correction
- Intercomparison between SAO OMI and OMPS formaldehyde retrievals
- Towards a long-term data record
- Next steps



Formaldehyde in the atmosphere: Formation of tropospheric ozone, organic aerosols, and tropospheric oxidation capacity



Formaldehyde in the atmosphere: sources and sinks



8/17/2017

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Formaldehyde in the atmosphere: satellite observations





(González Abad et al., AMT, 2016, doi:10.5194/amt-9-2797-2016)





Direct spectral fit of radiances

 $I = \left[(aI_o + \sum_i \alpha_i X_i) e^{-\sum_j \alpha_j X_j} + \sum_k \alpha_k X_k \right] ScalPoly + BasePoly$



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Direct spectral fit of radiances

Fitting window Radiance reference spectrum 327.7 nm - 356.0 nm

Computed online over the remote Pacific ocean between

 30° N and 30° S

3rd order

3rd order

Pre flight measurements

Chance and Kurucz (2010)

Chance and Orphal (2011), 300 K

Malicet et al. (1995), 228 K & 295 K

Vandaele et al. (1998), 220 K

Wilmouth et al. (1999), 228 K

Thalman and Volkamer (2013), 293 K

Chance and Spurr (1997)

Computed online (Chance et al., 2005)

Baseline polynomial Scaling polynomial Instrument slit function Solar reference spectrum H_2CO cross-sections O_3 cross-sections NO_2 cross-sections BrO cross-sections O_2-O_2 collision complex cross-sections Molecular Ring cross sections

Undersampling correction



Air mass factor correction

 $\Delta VCD = \frac{\Delta SCD}{AMF}$



Pacific Ocean Reference Sector Correction



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Pacific Ocean Reference Sector Correction





	Spectral Resolution [nm]	Spectral Coverage [nm]	Nadir Spatial Resolution [km ²]	Swath Size [km]	Overpass local time
OMPS	1.00	300-380	50 x 50	2800	13:30
OMI	0.42 (UV-2)	270-500	13 x 24	2600	13:42

Major differences between SAO OMPS and OMI formaldehyde retrievals

SAO retrieval	Fitting window [nm]	Surface Reflectance	Cloud parameters (cloud fraction and cloud pressure)
OMPS	327.7 – 356.0	TOMS climatology	Rotational Raman (Vasilkov et al., 2014)
OMI	328.5 – 356.5	OMI 5 year climatology (Kleipool et al., 2008)	O ₂ -O ₂ absorption (Stammes et al., 2008)



	Spectral Resolution [nm]	Spectral Coverage [nm]	Nadir Spatial Resolution [km ²]	Swath Size [km]	Overpass local time
OMPS	1.00	300-380	50 x 50	2800	13:30
ΟΜΙ	0.42 (UV-2)	270-500	13 x 24	2600	13:42





	Spectral Resolution [nm]	Spectral Coverage [nm]	Nadir Spatial Resolution [km ²]	Swath Size [km]	Overpass local time
OMPS	1.00	300-380	50 x 50	2800	13:30
OMI	0.42 (UV-2)	270-500	13 x 24	2600	13:42











Region	Correlation
Pacific Ocean	0.71
SEUS	0.99
Amazon	0.99
Europe	0.77
SE Asia	0.86
Tropical Africa	0.97
Southern Africa	0.95
East China	0.96

For these eight regions OMPS retrievals are biased high with respect to OMI retrievals 23%.

Towards a long-term data record



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Future work

- Reprocess whole data record with new L1B radiances, upgraded calibration and AMF calculation.
- Perform validation studies following Zhu et al., 2016 methodology (GEOS-Chem as intercomparison platform)
- Set up SAO public web page for data distribution

Campaign	Time Period	Location	Agency
TORERO	Jan. – Feb. 2012	Eastern Tropical Pacific	NCAR
DISCOVER-AQ	Jan. – Feb. 2013	California	NASA
NOMADSS	Jun. – Jul. 2013	Southeast U.S.	NCAR
SENEX	Summer 2013	Southeast U.S.	NOAA
DISCOVER-AQ	Aug. – Sep. 2013	Texas	NASA
SEAC ⁴ RS	Aug. – Sep. 2013	Southeast U.S.	NOAA
CONTRAST	Jan. – Feb. 2014	Western Tropical Pacific	NCAR
FRAPPÉ	Jul. – Aug. 2014	Colorado	NCAR
DISCOVER-AQ	Jul. – Aug. 2014	Colorado	NASA
WINTER	Jan. – Mar. 2015	Mid-Atlantic U.S.	NOAA
SONGNEX	Mar May 2015	Western U.S.	NOAA
KORUS-AQ	May – Jun. 2016	South Korea	NASA



Thanks for your attention



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8/17/2017

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DEVELOPMENT OF MULTI-SENSOR JPSS SO₂ PRODUCTS FOR VOLCANIC CLOUD MONITORING



Michael J. Pavolonis NOAA/NESDIS/STAR
Motivation



not depicted)

VOLcanic Cloud Analysis Toolkit (VOLCAT)



4). Volcanic Cloud Characterization



2017 JPSS Annual Meeting

5). Dispersion Forecasting



Example NRT Volcanic Ash Alerts from VOLCAT

Volcanic Cloud Alert Report

Date:	2017-08-15	
Time:	18:30:00	
Production Date and Time:	2017-08-15 20:18:05 UTC	
Primary Instrument:	NPP VIIRS	
More details V		

False Color Imagery (12–11µm, 11–8.5µm, 11µm) SNPP VIIRS (08/15/2017 – 18:30:00 UTC) SNPP VIIRS (08/15/2017 –

False Color Image (12-11, 11-8.5, 11) [zoomed-in]

Possible Volcanic Ash Cloud



Basic Information Volcanic Region(s) South America **Country/Countries** Ecuador Volcanic Subregion(s) Ecuador VAAC Region(s) of Nearby Volcanoes Washington **Identification Method** Plume Mean Object Date/Time 2017-08-15 18:34:06UTC Radiative Center (Lat, Lon): -2.010°, -78.340° Sangay (0.00 km) Licto (39.30 km) Nearby Volcanoes (meeting alert criteria): Tungurahua (60.90 km) Chimborazo (80.10 km) Quilotoa (142.80 km) Maximum Height [AMSL] 7.20 km; 23622 ft 90th Percentile Height [AMSL] 6.60 km ; 21654 ft Mean Tropopause Height [AMSL] 16.50 km ; 54134 ft Show More View all event imagery »

Sangay (not detected with ABI)

A). False Color Imagery (12–11μm, 11–8.5μm, 11μm) Terra MODIS (02/20/2001 – 08:45 UTC)

Weak Ash Signature

Strong Ash Signature

Weak Ash Signature

Pavolonis et al. (2015a); Pavolonis et al. (2015b)

Spatial Analysis: Cloud Objects Volcanic clouds, spectral metrics are used to

estimate ash probability

D IR Window Imagery and Ash Probability Terra MODIS (02/20/2001 – 08:45 UTC)

180 200 220 240 260 280 300 320 0.001 0.1 1 10 20 40 60 80 1 11 μm BT [K] Ash/Dust Probability [%]

2017 JPSS Annual Meeting

JPSS – Infrared Capabilities



BTD SO₂ = BT(1407.50 cm⁻¹) – BT(1371.25 cm⁻¹)

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VIIRS SO₂ Probability: Naïve Bayesian Classifier

A priori **Probability:** CrIS SO₂ BTD mapped to VIIRS swath and smoothed

Class Conditional Probabilities: Multivariate predictors trained using manual analysis of many volcanic events



The VIIRS predictors capture the influence of SO₂ absorption on 8.5 μ m and the lack there of at 11 and 12 μ m.

False Color Imagery (12–11µm, 11–8.5µm, 11µm) NPP VIIRS (09/03/2014 – 13:48:00 UTC)

Weak SO,

Signature

VIIRS SO₂ objects that contain spectrally robust VIIRS and/or CrIS SO₂ spectral signatures are selected

(09/03/2014 - 13:48:00 UTC)

VIIRS contributions are minimal in the northern parts of the SO₂ cloud

Strong SO

Signature

<figure><figure><page-footer>

IR Window Imagery and SO₂ Probability

Bogoslof (Alaska)



For well dispersed SO₂, OMPS and CrIS will have the greatest influence on results, but displaying SO₂ information on VIIRS images stills add value for users.

False Color Imagery (12–11μm, 11–8.5μm, 11μm) SNPP VIIRS (07/21/2017 – 08:36:00 UTC)

Iztaccihu

Popocatepeti

Jocohillan



Chichinautzin

Low level SO₂ plume





Malinche, La

Annotation Key (annotation colors are not related to colors in underlying image) Ash/Dust Cloud Volcanic Cb Thermal Anomaly

False Color Imagery (12–11μm, 11–3.9μm, 11μm) SNPP VIIRS (07/21/2017 – 08:36:00 UTC)

Pana

Iztaccinuat

Popocatepeti

Chichinautzin

Jocolitlan

Toluca, Nevado de

Feature is not present in imagery that does not include SO₂ absorption channels





Malinche, La

Annotation Key (annotation colors are not related to colors in underlying image) Ash/Dust Cloud Volcanic Cb Thermal Anoma

Spatial – Geometric Properties

Most everyday volcanic ash emissions have a weak multi-spectral signature. They are identifiable in imagery due to the combination of spectral signature and plume like shape.









Automated Volcanic Cloud Time Series



Collaboration

Matt Pritchard (Cornell) - PI Mike Poland (USGS) - PI **Ben Andrews (Smithsonian)** Juliet Briggs (U. Bristol) Simon Carn (Mich. Tech) Julie Griswold (USGS) **Brenda Jones (USGS)** Sue Louglin (British Geological Survey) Taryn Lopez (UAF) Paul Lindgren (JPL) Franz Meyer (UAF) Mike Pavolonis (NOAA) Ivan Petiteville (ESA) **Kevin Reath (Cornell) Dave Schneider (USGS)** Greg Vaughan (USGS) **Christell Wauthier (Penn St.) Rick Wessels (USGS)** Rob Wright (U. Hawaii)

USGS Powell Center



Ongoing Work

So Far: Primary focus on accurately quantifying the horizontal bounds of volcanic SO₂ clouds Continuing Work: Incorporation of OMPS, merged SO₂ loading estimates, merged SO₂ alerts and time series (including GOES-R) User interactions: Close relationship with NOAA VAAC's, USGS, and many international partners

Other Collaborations: NOAA ARL (HYSPLIT) group

References

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