Expanding the suite of composition products from the NASA sounders

Vivienne Payne[1], Susan Kulawik[2], Dejian Fu[1], Kevin Bowman[1], John Worden[1], Jessica Neu[1], Karen Cady-Pereira[3], Helen Worden[4], Gene Francis[4], Ming Luo[1], Matt Alvarado[3]

1. Jet Propulsion Laboratory, California Institute of Technology
2. BAERI/NASA Ames
3. AER
4. NCAR

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Tropospheric composition from satellites

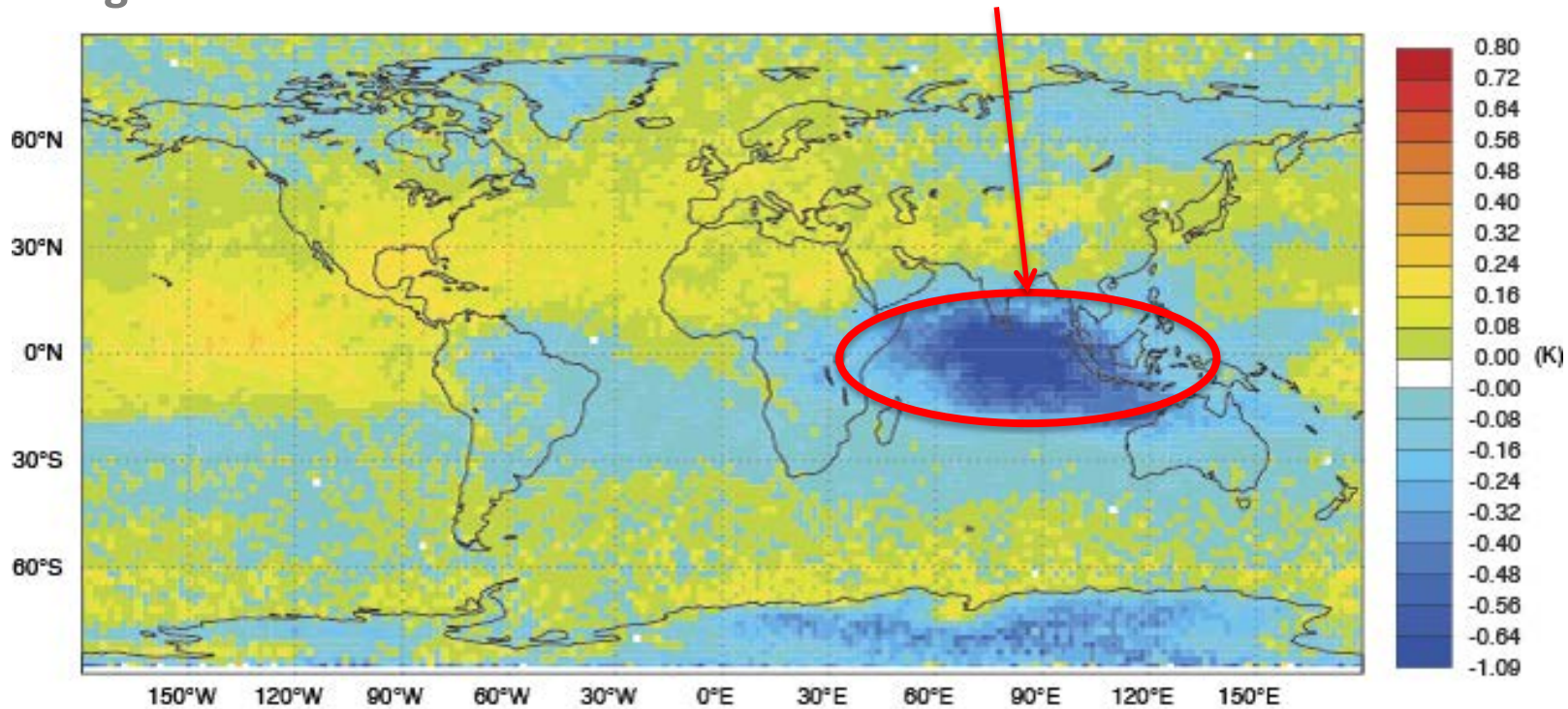
- Satellite measurements of tropospheric composition can further our understanding of
  - Air quality, long-range pollution transport
  - Radiative forcing/climate
  - Water, carbon, nitrogen cycles
- Global-scale, long-term measurements

- Impacts of trace gas signatures on radiance bias correction for NWP (see next slide)
- Impact on channel selection for NWP?

Hydrogen Cyanide (HCN) signal in TIR radiances

Figure: ECMWF

Radiance bias associated with HCN



Bias in observed minus calculated METOP-A IASI radiances at 713 cm^{-1}

Monthly mean values, 15th September to 15th October 2015

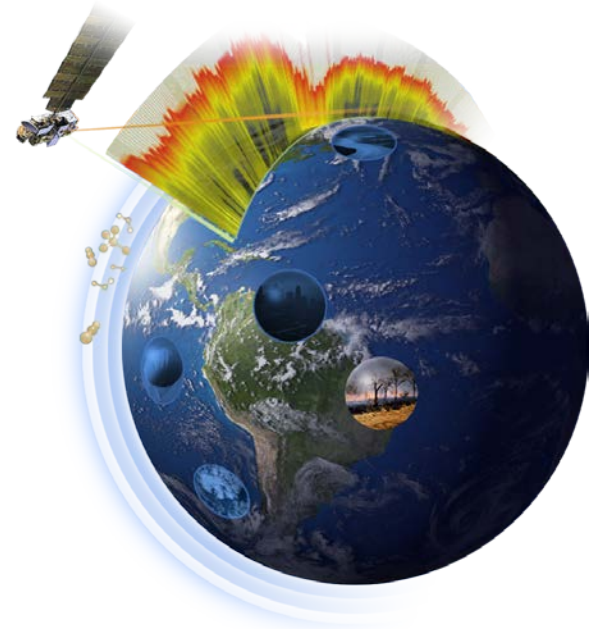
http://www.ecmwf.int/en/about/media-centre/news/2015/weather-satellites-pick-indonesian-fire-signal-over-indian-ocean

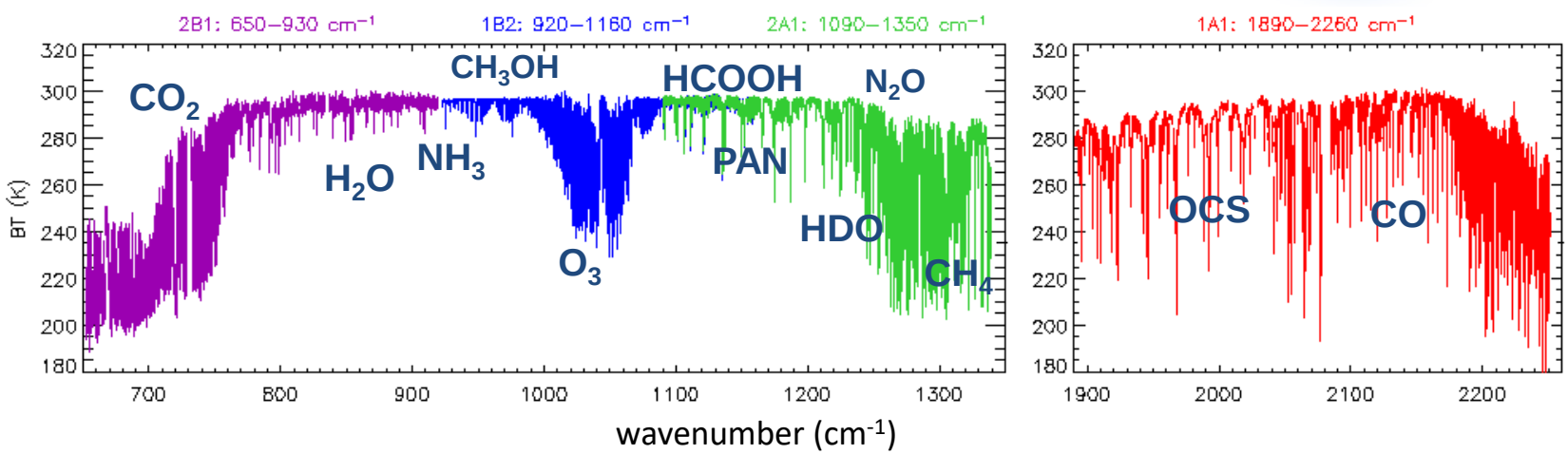
Community workshops

- **2010:** NASA Community Workshop on Polar Orbiting IR and MW sounders
- **2014**: CrIS Atmospheric Chemistry Data User's Workshop
- **2014**: NASA Ames Workshop on Outstanding Questions in Atmospheric Composition, Chemistry, Dynamics and Radiation for the Coming Decade
- Recommendations include:
  - Formation of a US-based Sounding Team
  - **Continuity** of EOS records, including composition
  - Observation of **multiple species**, including
    - O_3, CH_4, NO_x, CO, PAN, NH_3, N_2O, HNO_3, VOCs
  - Role of models in analysis of measurements of atmospheric composition
    - Observations must have well-characterized errors
    - Observation operator (averaging kernel) should be supplied for each observation.

The Aura Tropospheric Emission Spectrometer

- **Aura**: Earth Observing System satellite
  - **Focused on composition**
  - ozone, air quality and climate
- **Tropospheric Emission Spectrometer (TES)**
  - Fourier Transform Spectrometer
  - +/- 8.3 cm optical path difference
  - **~0.1 cm^{-1}** spectral resolution





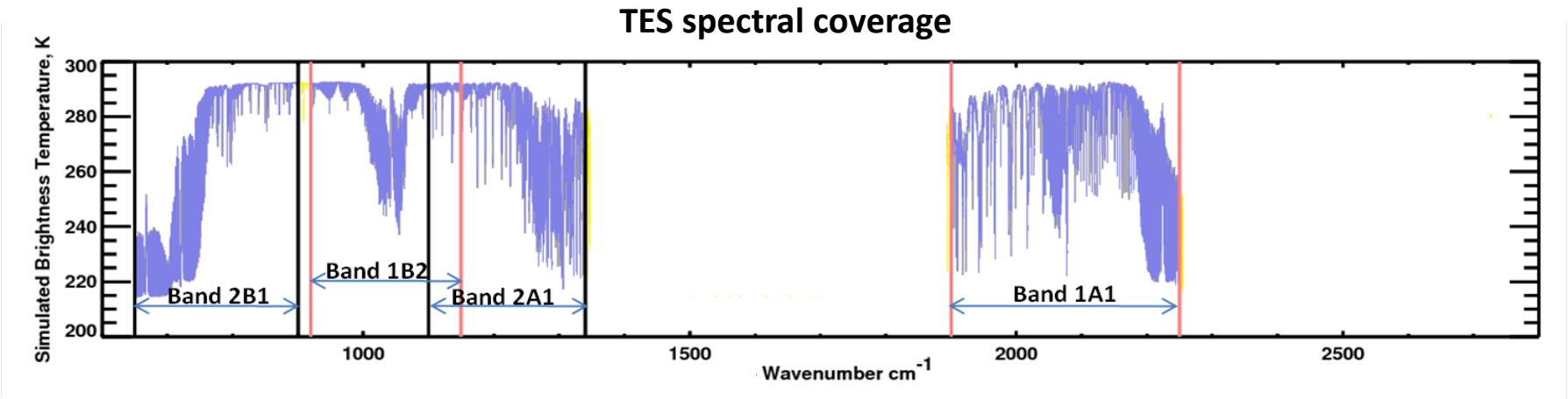
Optimal estimation retrievals

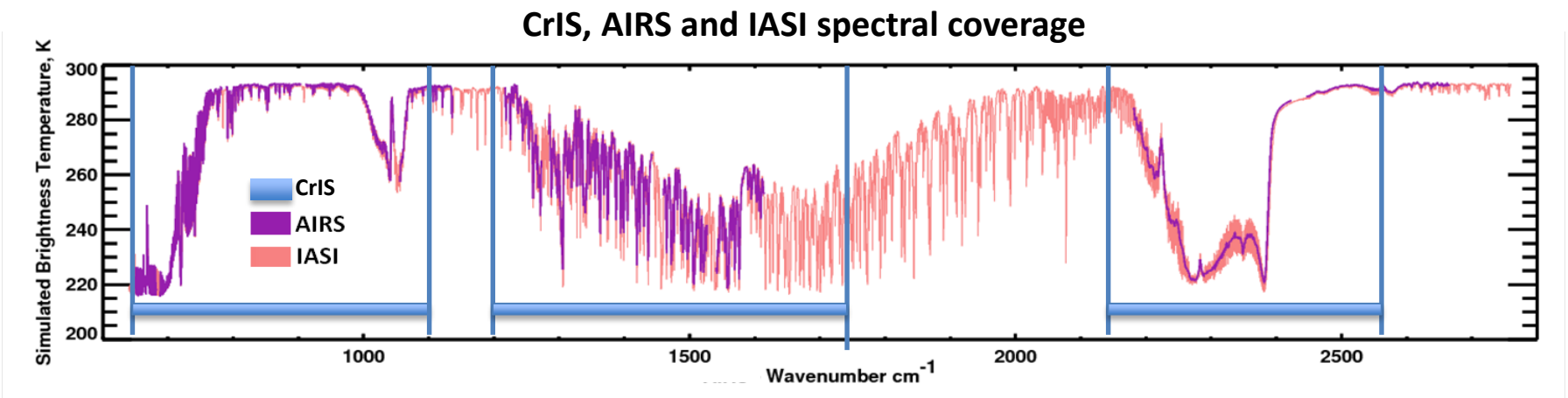
- Advantages of optimal estimation approach
  - Error estimates
  - Sensitivity diagnostics (averaging kernels)
- TES algorithm: Bowman et al. [2006]
- MUSES: See Dejian Fu's talk

From CrIS Atmospheric Chemistry Data Users' Workshop

- Importance of communication/collaboration between retrieval developers and user community
- **Recommendation:**
  - **Supply user-friendly "Lite" files**
    - Arranged by date, not by granule/orbit
    - Full diagnostic information on reduced levels
    - With ancillary info (e.g. post-processing/T700)
    - Available for TES and OCO-2

Spectral coverage of TIR sounders





Available trace gas products from **NASA/NOAA** thermal-IR sounders*

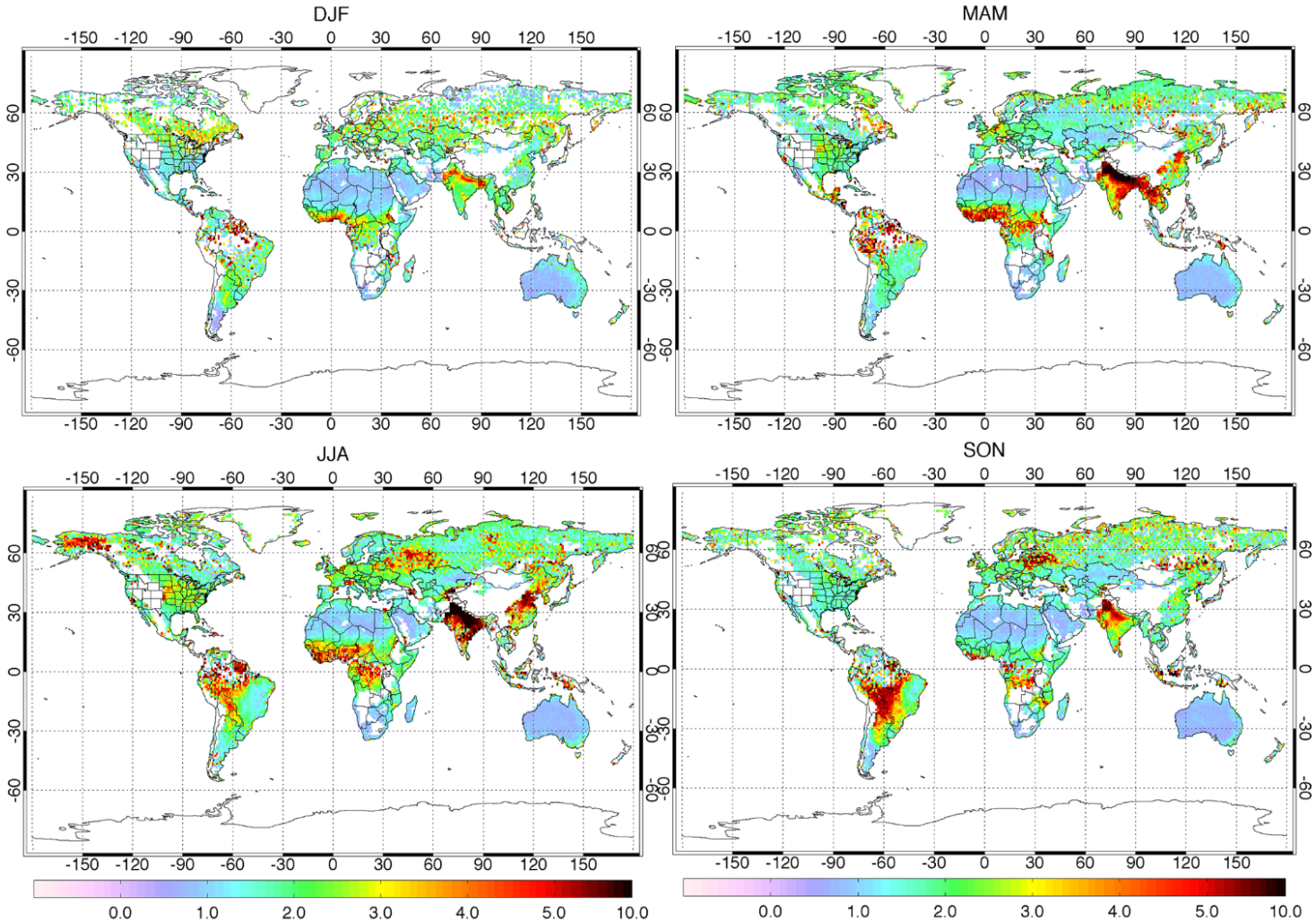
	Molecule	AIRS v6	AIRS OE J. Warner et al	AIRS NUCAPS	TES v7	CrIS NUCAPS	CrIS AER/NCAR+
Omnipresent	O_3	Y		Y	Y	Y	
	CO	Y	Y	Y	Y	Y	+
	CH_4	Y		Y	Y	Y	
	CO_2	Y		Y	Y	Y	
	N_2O		Y	Y	Y	Y	
	HDO				Y		
	HNO_3		Y	Y		Y	
	OCS	AIRS gap	AIRS gap	AIRS gap	Y	CrIS gap	CrIS gap
Observable at enhanced concentrations	NH_3		Y		Y		+
	CH_3OH				Y		
	HCOOH	AIRS gap	AIRS gap	AIRS gap	Y	CrIS gap	CrIS gap
	PAN				Y		
	SO_2	flag		Y		Y	

*Attempt to capture range of products avail – please excuse omissions/misunderstandings
+ Not yet publicly available, but will be in forseeable future

13 years of NH_3 from AIRS

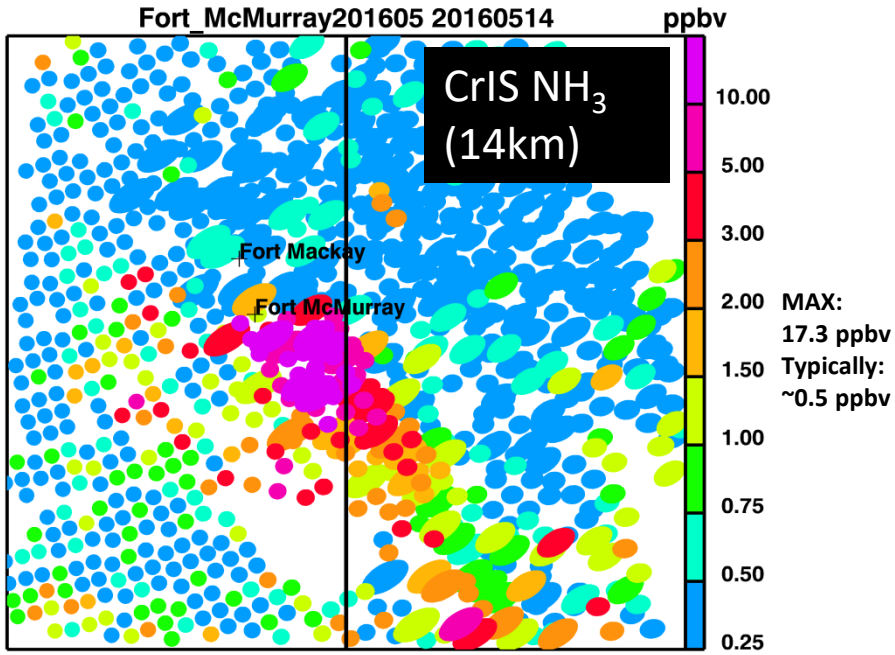
Warner et al., ACP [2016] – Optimal estimation retrievals

Retrievals on cloud-cleared radiances: 45 km^2 pixel size



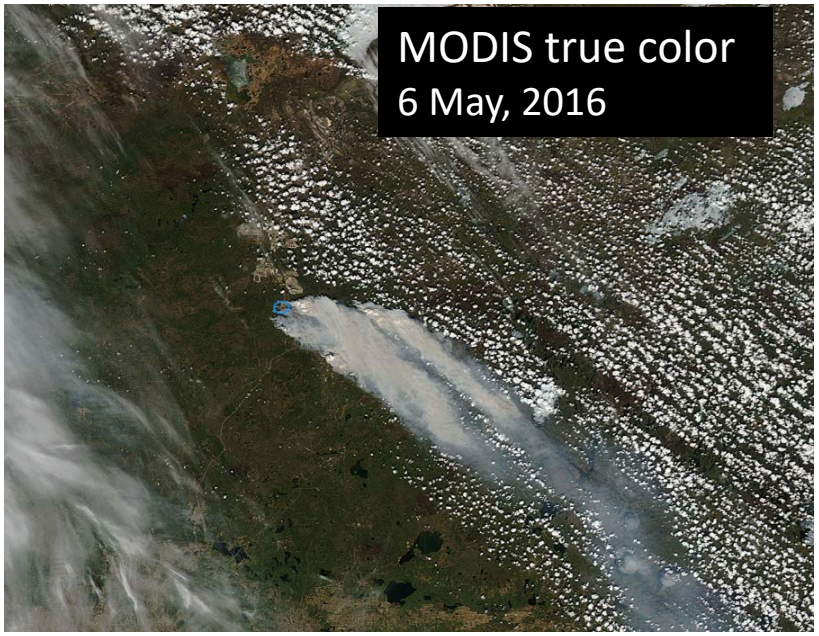
Examples of SNPP-CrIS NH_3 and CO from Ft. McMurray fires in Alberta, May 2016

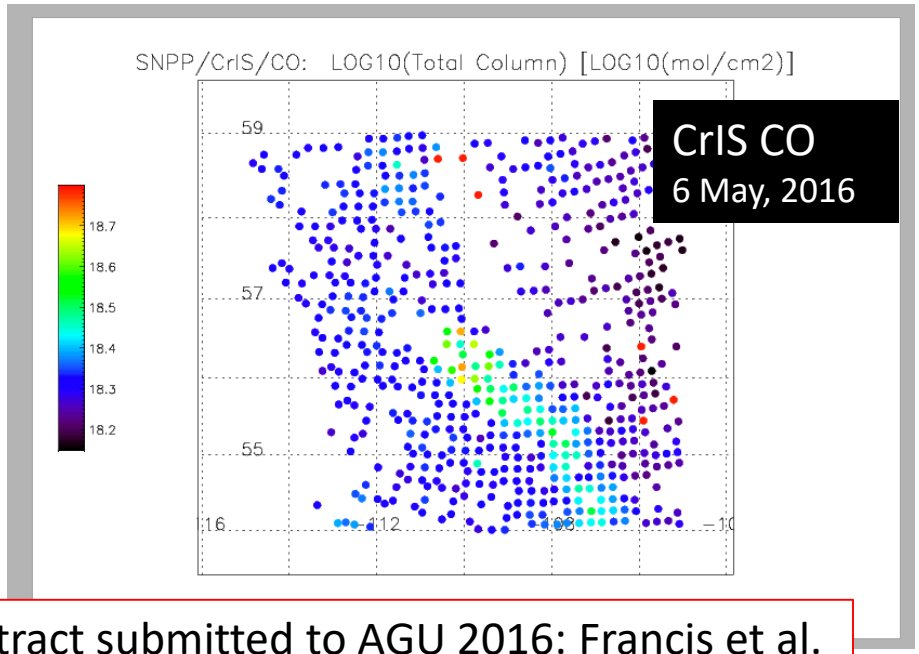
(K. Cady-Pereira, H. Worden, G. Francis)



Optimal estimation retrievals
Retrievals performed on single FOVs

Delivery to SIPS:
- NH_3 planned for January 2017
- CO: TBD, mid-2017 reasonable





Abstract submitted to AGU 2016: Francis et al.

Peroxyacetyl Nitrate (PAN)

- PAN: Reservoir for NO_x radicals, Important for long-range transport of pollution
  - Formed from (anthropogenic/lightning/fire) NO_x in the presence of **VOCs**
- PAN from TES has been used in studies of fire anthropogenic and lightning sources, and of seasonal variations in pollution transport
  - Payne et al. [2014]; Zhu et al. [2015]; Payne et al. [2015]; Jiang et al. [2016]; Zhu et al. [2016]; Fischer et al. [2016]
- TES PAN retrievals use feature at **1140-1180 cm^{-1}** (falls in AIRS/CrIS spectral gap)
- Possible alternative for AIRS/CrIS: Use feature at **780-810 cm^{-1}**

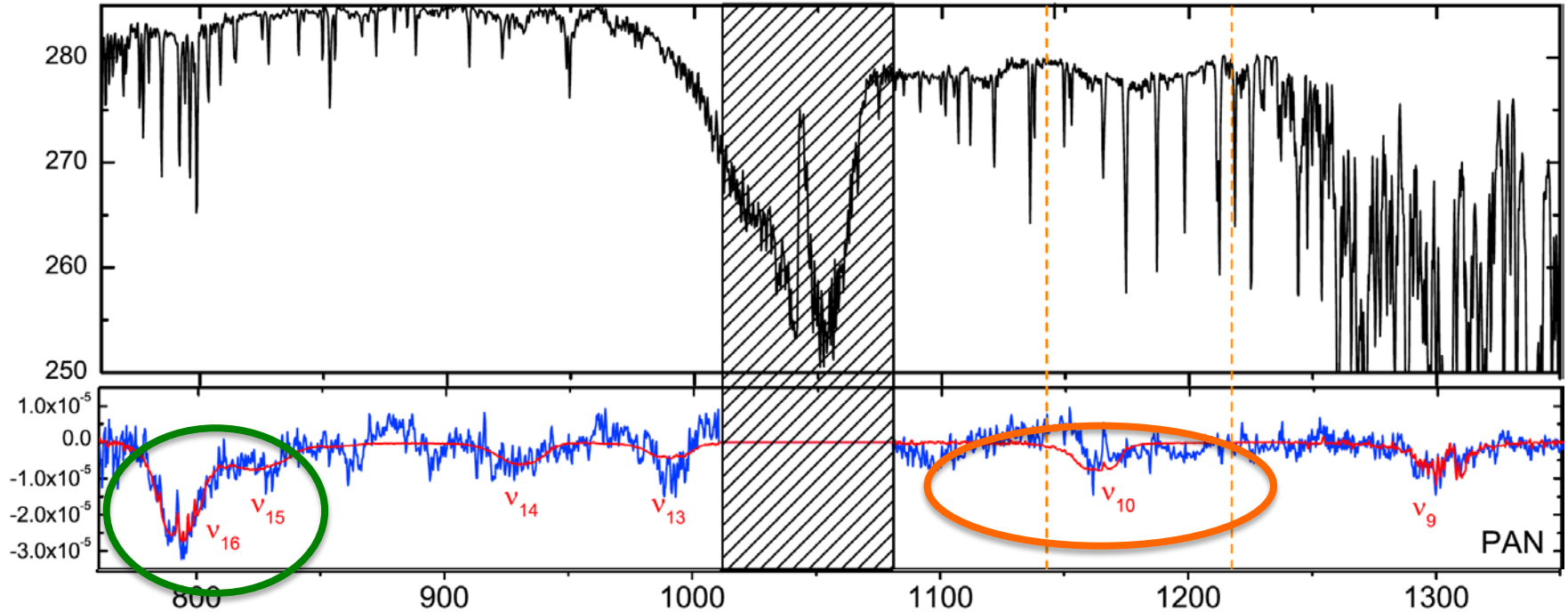
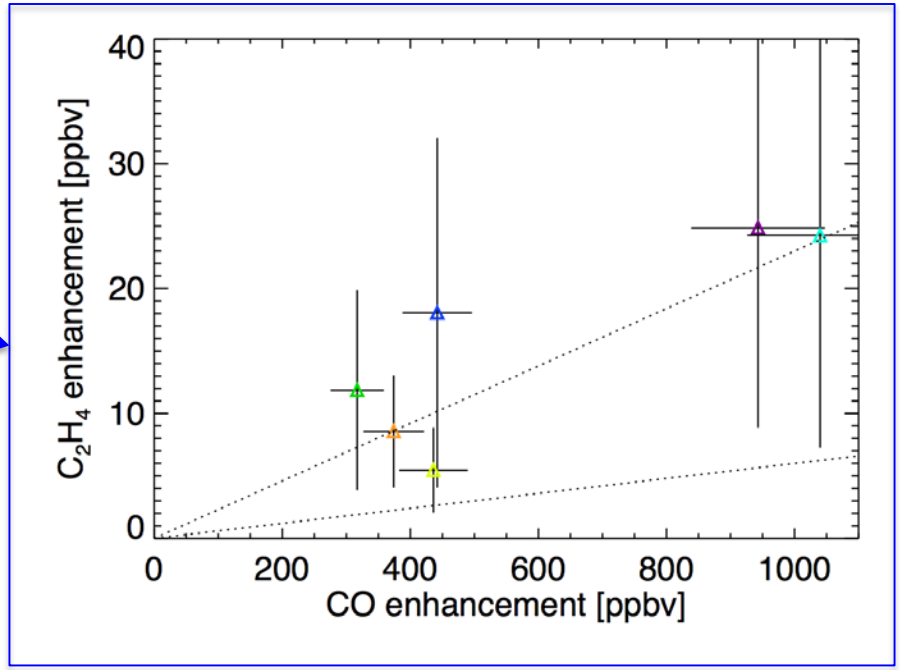


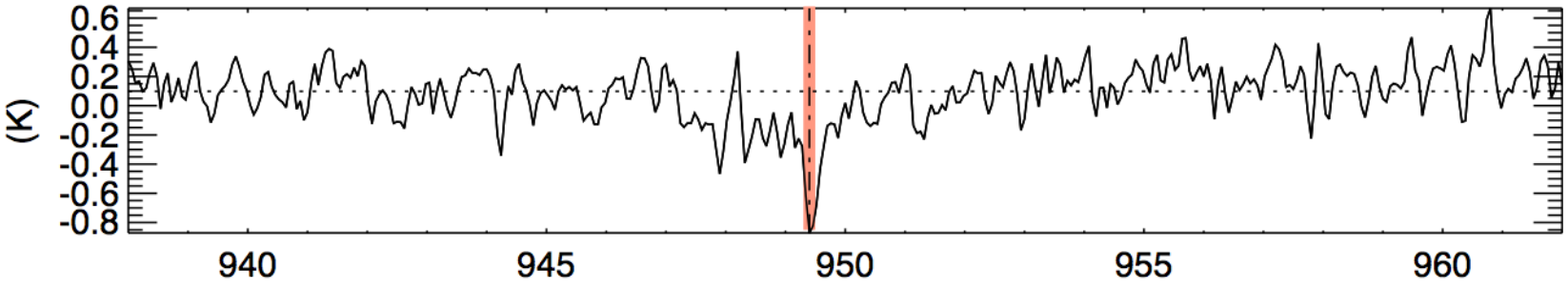
Figure from Clarisse et al. [2011]

Volatile organic compounds (VOCs): Ethylene (C_2H_4)

- Fire, anthropogenic and biogenic sources
- TES observations of C_2H_4 in fire plumes
  - Alvarado et al. [2011]: Single fire plume
  - **Dolan et al. [2016]: Multiple fire plumes**



- Future work:
  - Assess signals from oil refinery regions
  - Assess signals from biogenic sources



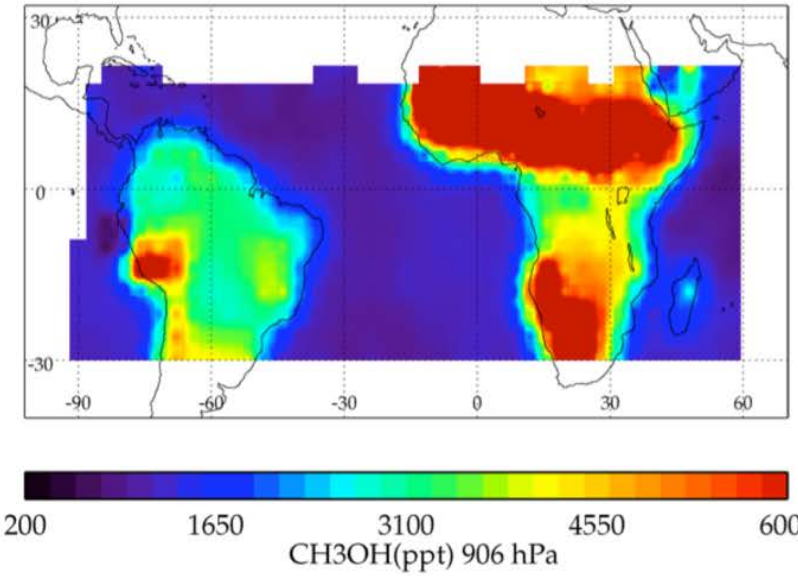
Volatile Organic Compounds (VOCs):

Methanol (CH_3OH) and **acetone** (CH_3-CO-CH_3)

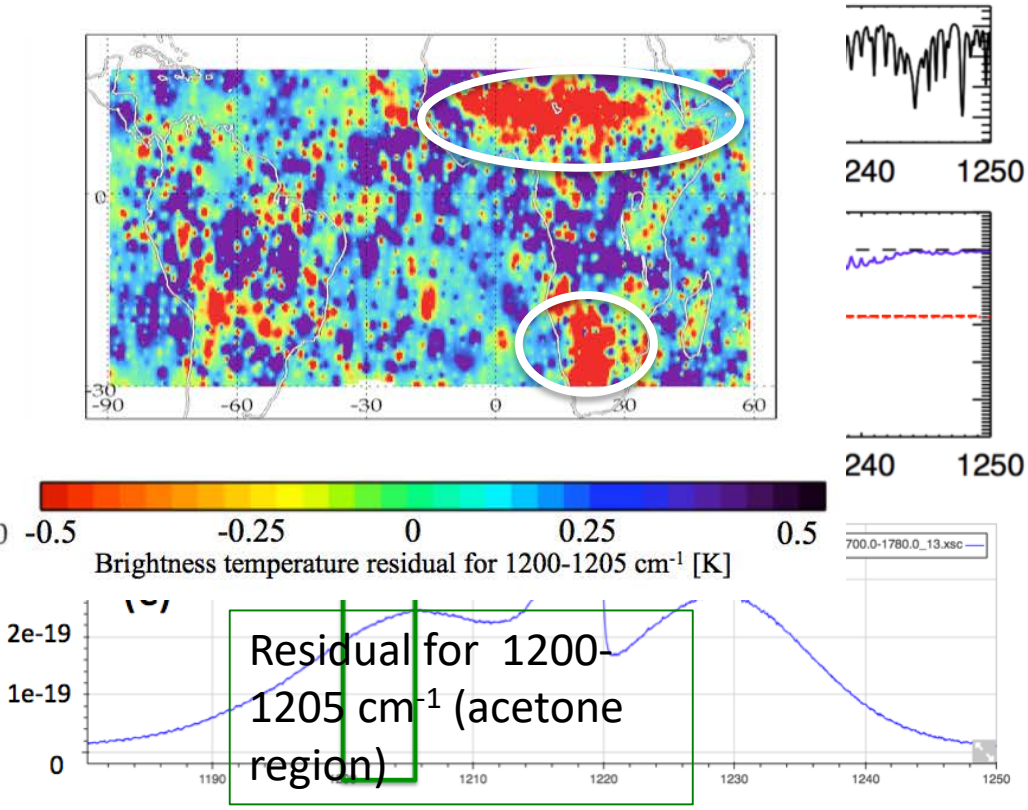
Existing TES product

Under investigation

- Biogenic, fire and anthropogenic sources



TES methanol for January 2009



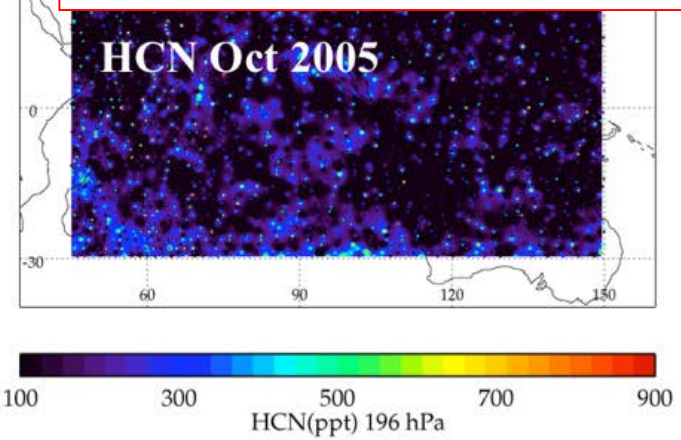
Residual for 1200-1205 cm^{-1} (acetone region)

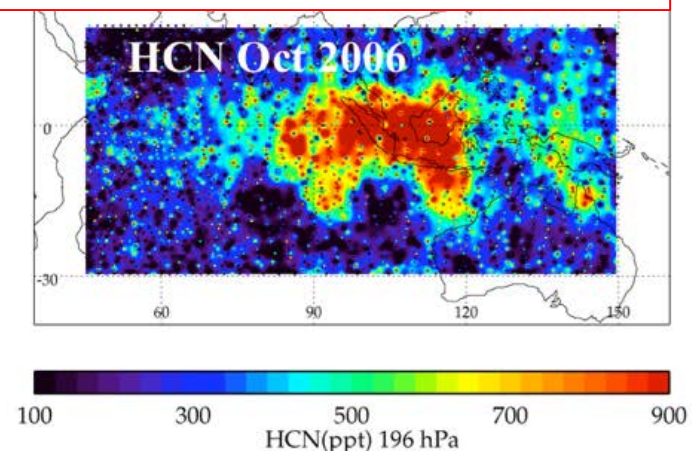
Spectral signature of acetone

Hydrogen Cyanide (HCN)

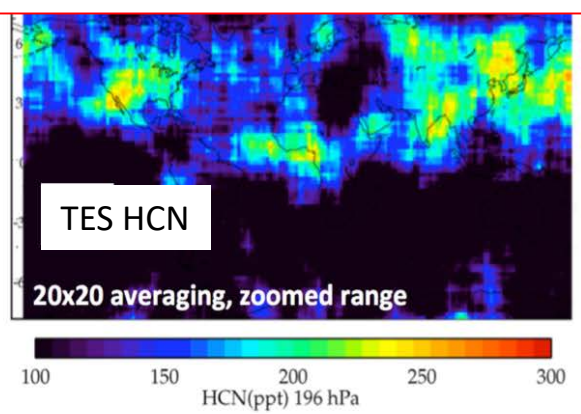
- Tracer of biomass burning influence
- IASI HCN retrievals: Duflot et al. [2015]
- New TES results (S. Kulawik et al., presented at Aura STM 2016):

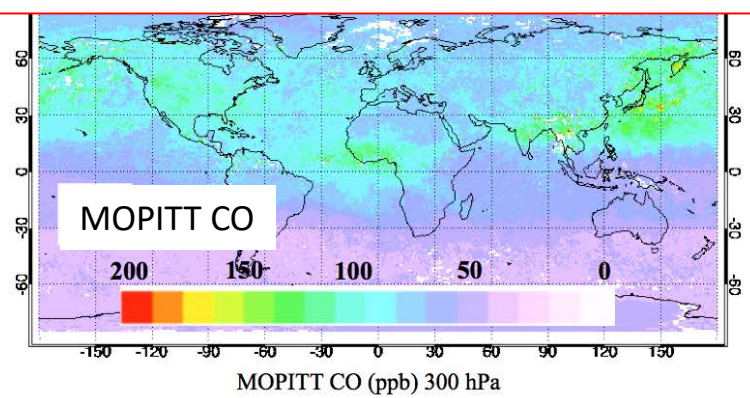
Extreme case: 2006 Indonesian fires: Maps of single footprint results



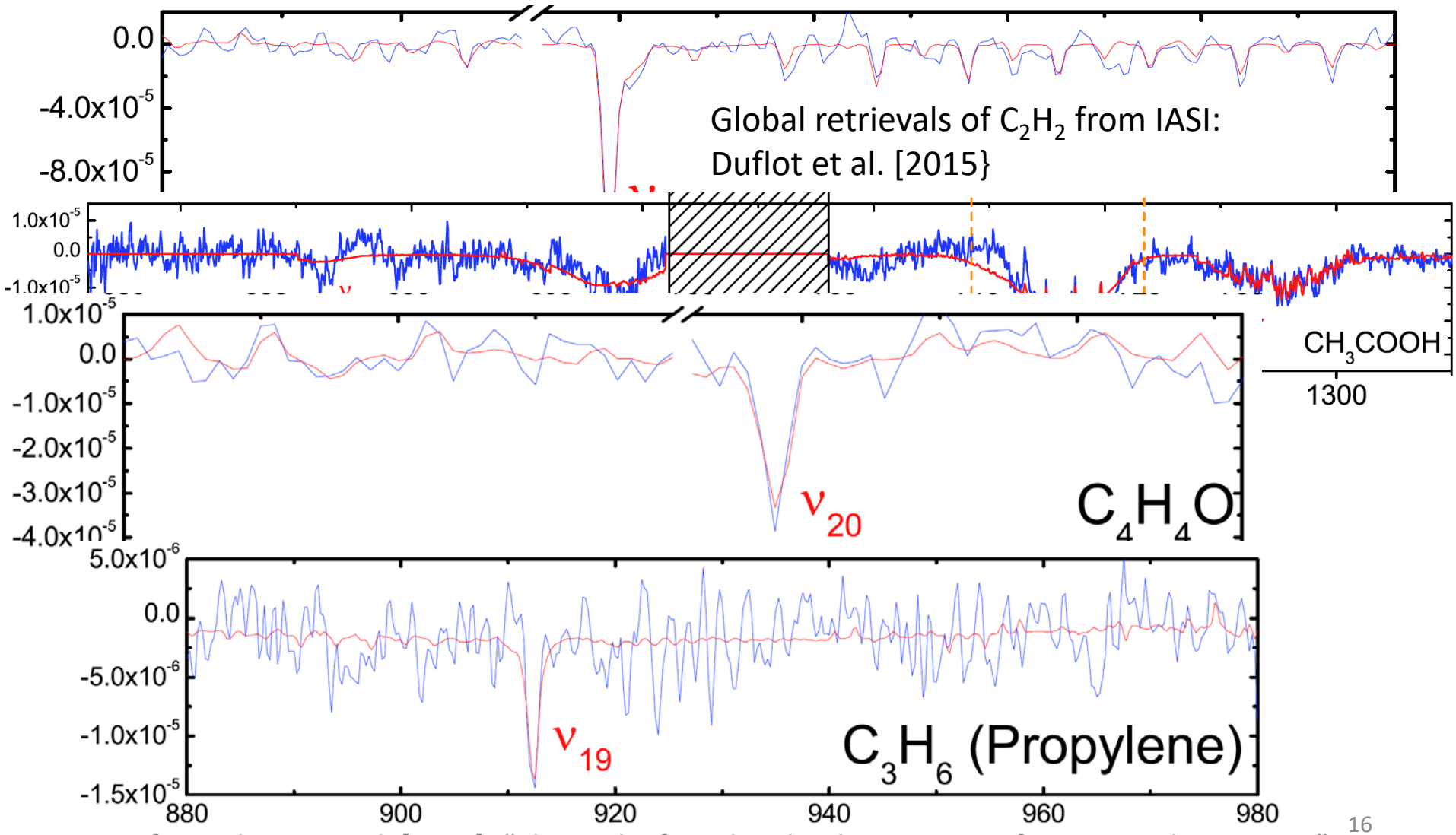


For less extreme conditions, averaging is needed to discern large-scale spatial features





The list goes on….



Figures from Clarisse et al. [2011], "Thermal infrared nadir observations of 24 atmospheric gases"

Validation is needed throughout the span of the data record

- Importance of **profile measurements** for validation of TIR retrievals
  - **TIR does not measure the total column!**

- Tropospheric composition activities at NASA
  - History of aircraft campaigns targeting composition
- NOAA composition activities
  - Incudes upcoming FIREX campaign

- Value of HIPPO for validation of long-lived species
  - Examples: Wecht et al. [2012]; Xiong et al [2013]; Frankenberg et al. [2016]
- Value of ground-based FTIR measurements
  - Example: Dammers et al. [2016]; Duflot et al. [2015]

- **Limited validation data available for minor species**
- **Short-lived species are particularly difficult to validate**

- **Indirect validation using chemistry transport models**
  - **Compare ($obs_{validation}$ – model) with ($obs_{satellite}$ – model)**
  - Example: Wells et al. [2012]

Summary

- Satellites provide **global-scale** measurements over **multiple years**
- Understanding ongoing changes in tropospheric composition
  - Measurements of **multiple trace gases** needed to provide constraints on chemistry-transport models
- **Thermal IR sounder data contain a wealth of information**
  - Air quality, long-range pollution transport
  - Radiative forcing/climate
  - Water, carbon, nitrogen cycles
- **Continuity of EOS-era records is important**
  - Ongoing validation against independent measurements is needed
- **Thermal IR sounder data have not yet been fully mined**
  - Potential for development of **multiple new products**
- Importance of **sensitivity diagnostics** and well-characterized errors to ensure extensive use within the wider community

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• **Bowman et al. [2006]** Tropospheric Emission Spectrometer: Retrieval Method and Error Analysis, *IEEE Trans. Geosci. Remote Sensing, 44*, 1297- 1307

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• **Dolan et al. [2016]** Satellite observations of ethylene (C_2H_4) from the Aura Tropospheric Emission Spectrometer: A scoping study, *Atmos. Env.*, 141, 388-393

• **Duflot et al. [2015]** C2H2 and HCN from IASI satellite observations: global distributions, validation and comparison with model

• **Fischer et al. [2016]** Summertime free tropospheric PAN over the U.S. as observed by TES ad simulated by GEOS-Chem, Presentation at the Aura Science Team Meeting, Rotterdam

• **Frankenberg et al. [2016]** Using airborne HIAPER Pole-to-Pole Observations (HIPPO) to evaluate model and remote sensing estimates of atmospheric carbon dioxide, Atmos. Chem. Phys., 16, 7867-7878

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• **Xiong et al. [2013]**, Mid-upper tropospheric methane retrieval from IASI and its validation, Atmos. Meas. Tech., 6, 2255–2265

• **Zhu et al. [2015]** TES observations of the interannual variability of PAN over Northern Eurasia and the Relationship to Springtime Fires, *Geophys. Res. Lett*.

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Back-up slides on AER/NCAR NH_3 and CO

CrIS NH_3 and CO

Karen Cady-Pereira, AER
Helen Worden & Gene Francis, NCAR

NH_3 Status

- NH_3 Prototype developed from TES NH_3 algorithm
- Similar microwindows
- Same three a priori profiles and constraints
- Optimal estimation using OSS as forward model
- First step is an emissivity/surface temperature retrieval
- Currently the driver and the retrieval use a mix of IDL/Perl codes
- Later this year we will switch to using AER's updated ESDR code for the retrieval
- Will experiment with adding a cloud optical depth retrieval or using VIIRS cloud mask

NH_3 Status (cont.)

- Retrievals use radiances from every FOV, water vapor and temperature from each FOR
- High spatial resolution very important for a highly reactive and thus highly variable gas like NH_3.
- Algorithm has been extensively run:
  - Colorado DISCOVER-AQ
  - SENEX
  - Fort McMurray fires
- Code will be delivered as a separate package from the AER water vapor/temperature retrieval
- Delivery to the SIPS is planned for January 2017

CO Status

- Prototype CrIS CO retrieval code at NCAR has been extended to process high-resolution CrIS spectra.
  - "high-res" processing code has been debugged and is running successfully.
- incorporates previously-developed MOPITT-based covariance matrix calculations.
- Initial hi-res CO micro-window assignments made.
- Hi-res CrIS CO retrievals successfully carried out over the Fort McMurray, Canada, fires for 6 May 2016
  - Retrievals with low res. CO were also tested for central valley, CA

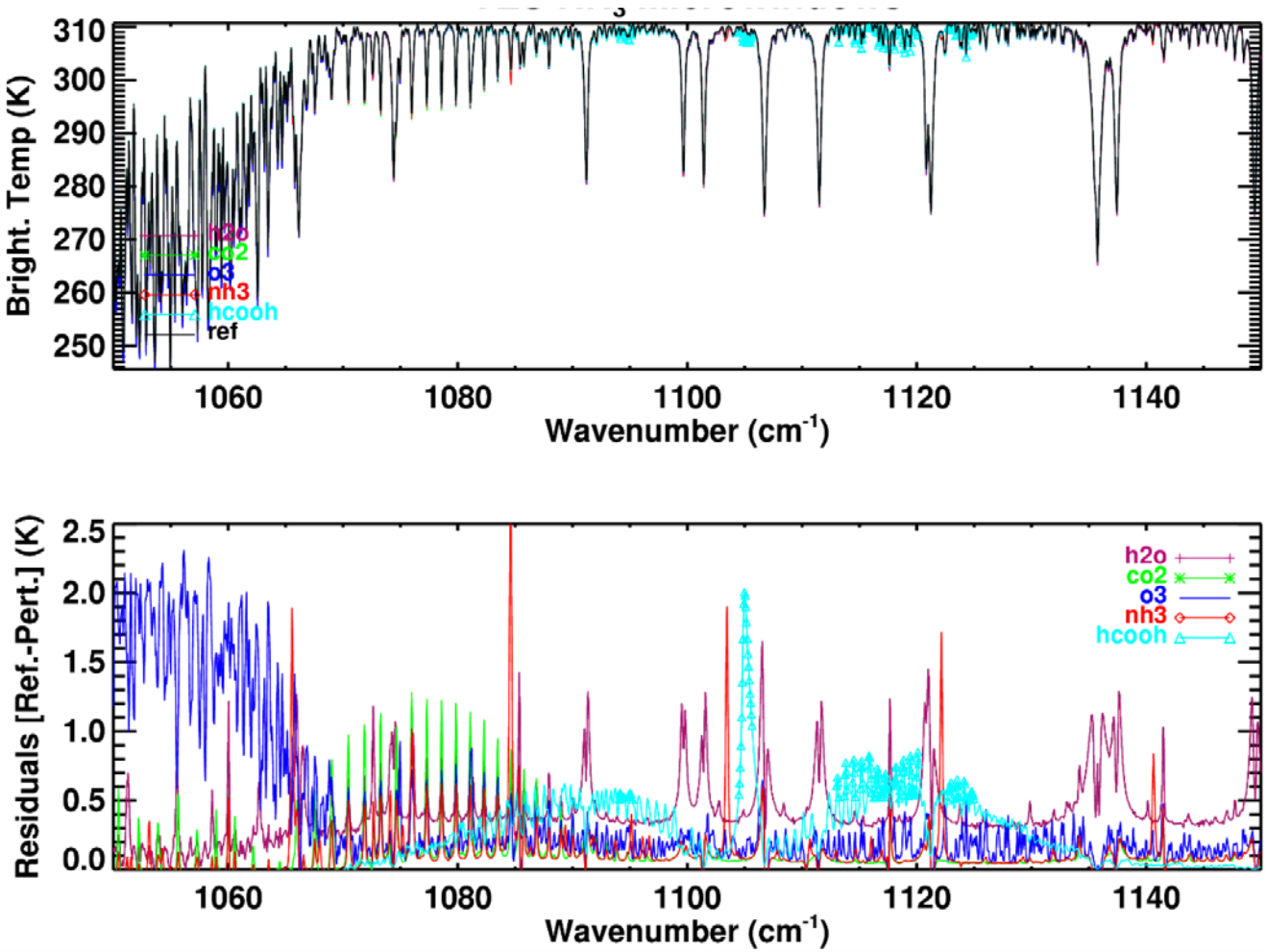
CO Status (cont.)

- Hi-res retrievals exhibit a high-percentage convergence fraction, reasonable optimal-estimation averaging kernels, and reasonable degrees-of-freedom figure of merit.
- Need to include cloud screening (same as for NH_3).
- Delivery to the SIPS is TBD, but mid-2017 is reasonable.
- Abstract submitted to 2016 Fall AGU Meeting:

  Title: Toward a multi-decadal record of satellite CO from MOPITT to Suomi NPP/CrIS: Overview and Initial Results Authors: Gene Francis (NCAR), Karen Cady-Pereira (AER), Helen Worden (NCAR), Mark Shephard (EC), Dejian Fu (JPL)

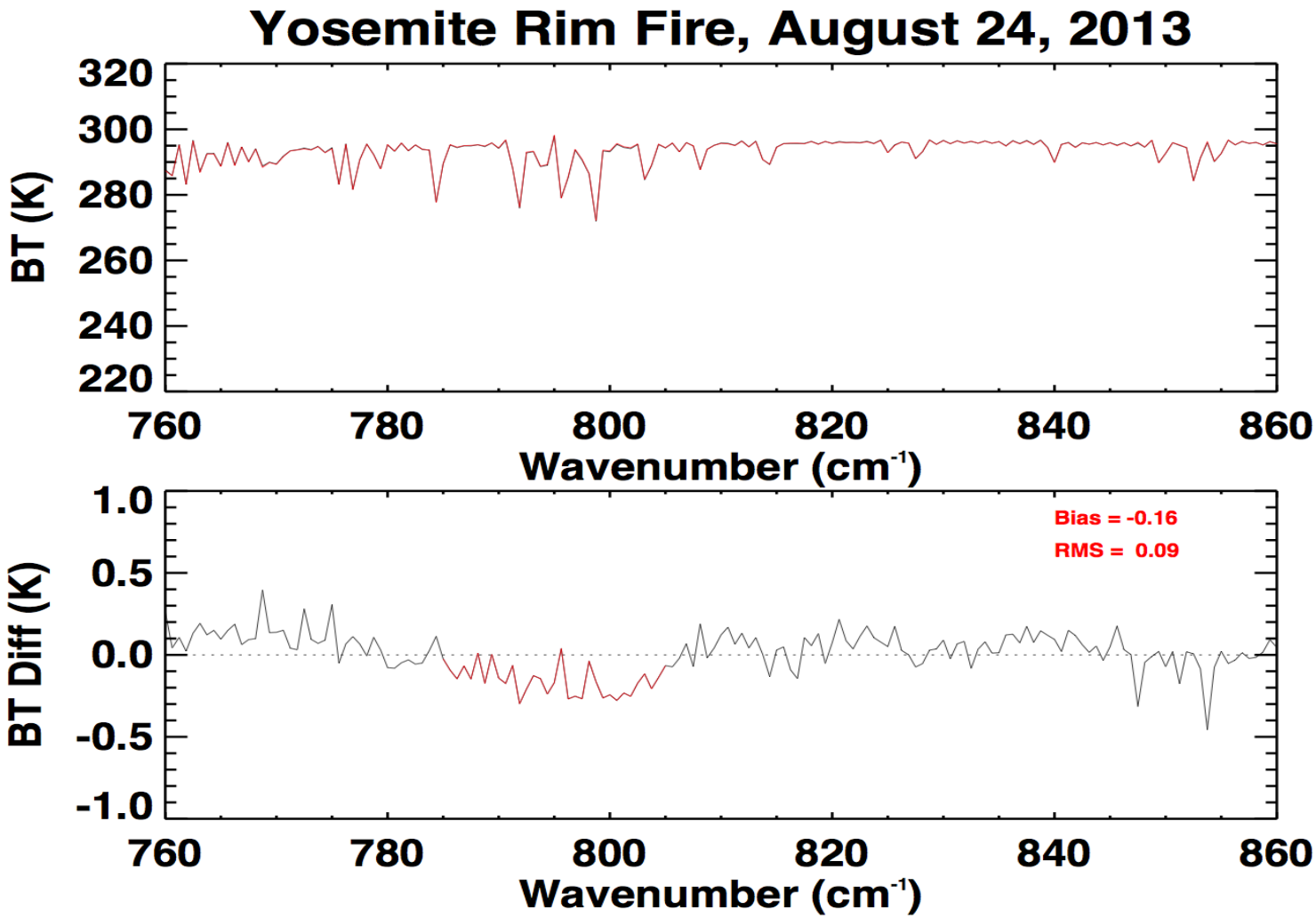
Back-up slides on other species

Formic acid (HCOOH)



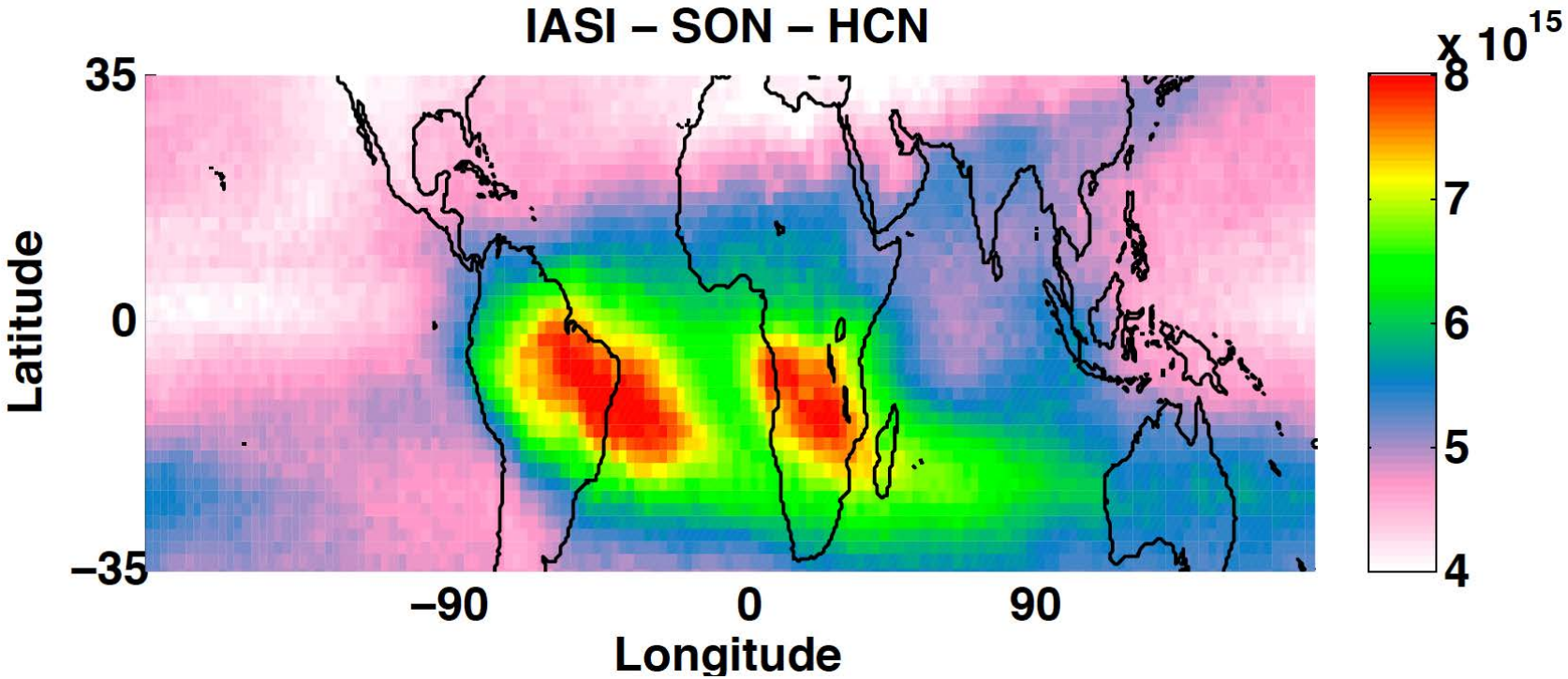
Cady-Pereira et al. [2015]

PAN from CrIS

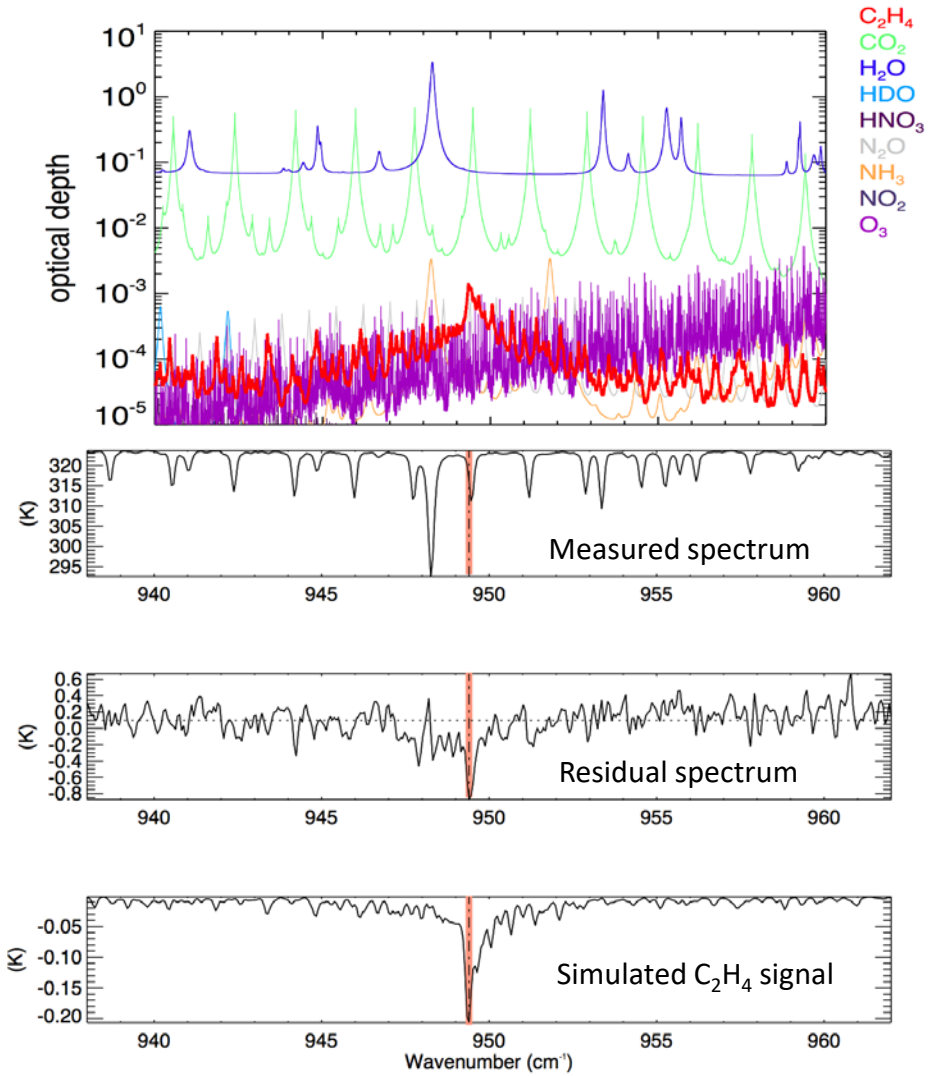


Hydrogen Cyanide (HCN)

- Highlighted in the Workshop report
- Tracer of biomass burning influence
- IASI HCN retrievals: Duflot et al. [2015]

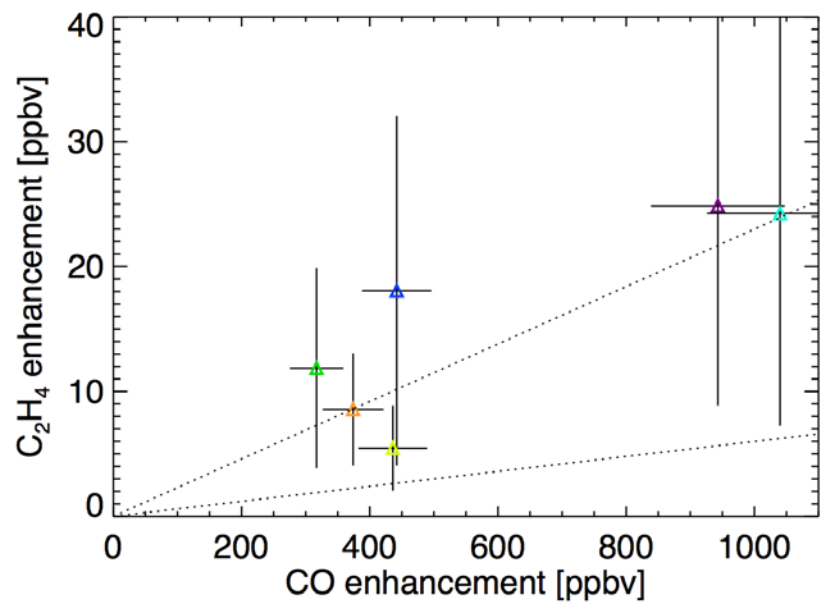


Ethylene (C_2H_4)



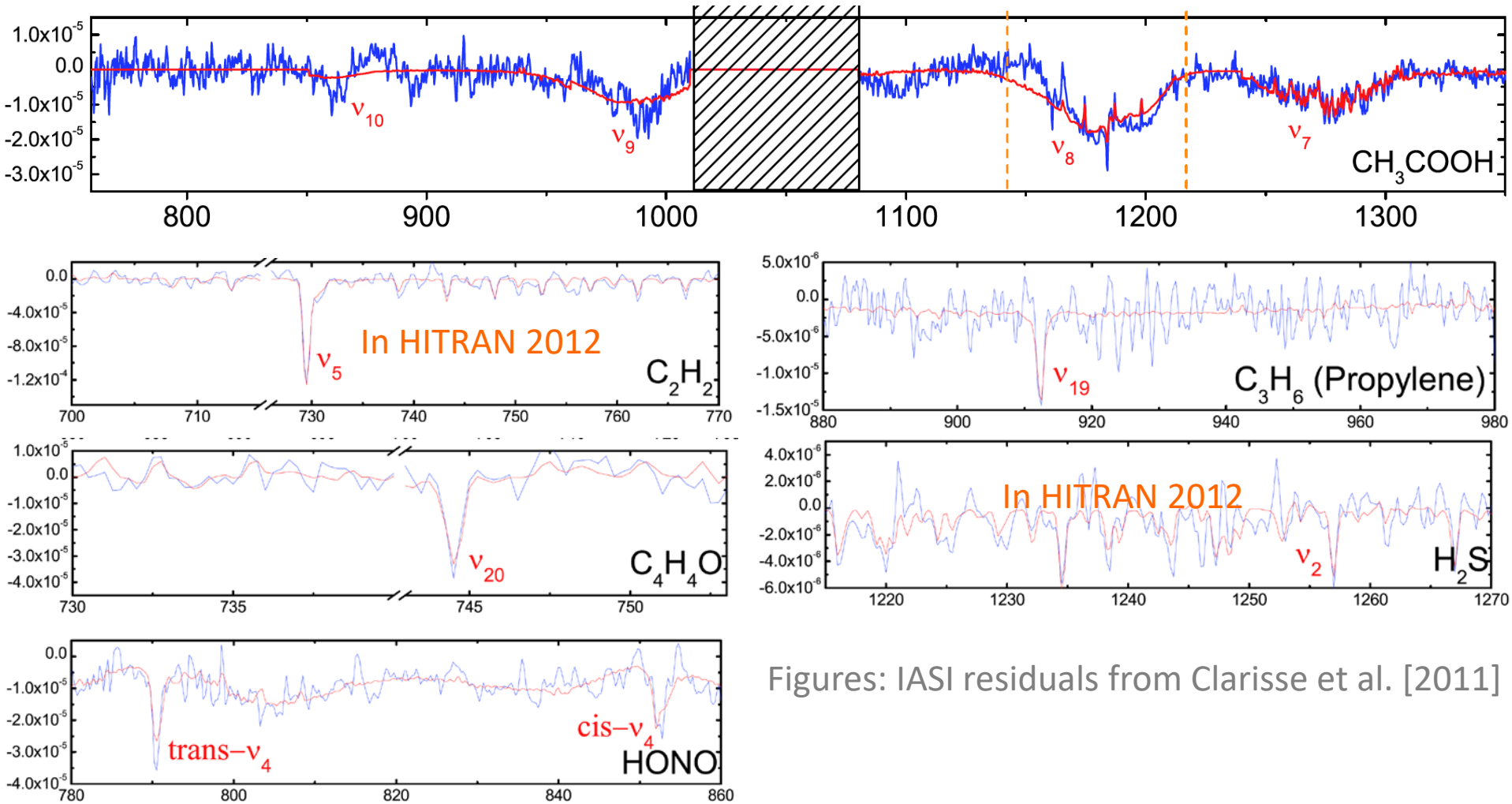
Highlighted in the CrIS Workshop report
Associated with production of O_3 and its precursors
Detection and measurement:

- TES:
  - One fire plume: Alvarado et al. [2011]
  - Multiple fire plumes: Dolan et al. [2016]
- CrIS:
  - Karen Cady-Pereira's talk last year



Figures from Dolan et al. [2016]

More possibilities….



Figures: IASI residuals from Clarisse et al. [2011]