Evaluation of sounder composition products

Vivienne Payne

Jet Propulsion Laboratory, California Institute of Technology

Acknowledgements

- Bill Irion (JPL/Caltech)
- Susan Kulawik (BAERI/NASA Ames)
- AIRS team at JPL
- Ruth Monarrez, Evan Manning and the Sounder SIPS team
- Nadia Smith, Chris Barnet (STC)
- Kevin Bowman, John Worden (JPL/Caltech)
- NASA Sounder Science Team
- Kazu Miyazaki (JAMSTEC)
- Mark Parrington (ECMWF)

	Omnipresent									Observable at enhanced concentrations					
Molecule	O_3	O_3 IRKs	CO	CH_4	CO_2	N_2O	HDO	HNO_3	OCS	NH_3	CH_3OH	HCOOH	PAN	SO_2	Isoprene

Sounder composition products

- Long term records
- Product-centric rather than instrument-centric
- Importance of sensitivity diagnostics and error characterization

- Perspectives
  - Evaluation for AIRS v7 algorithm
  - Wider Sounder Science context

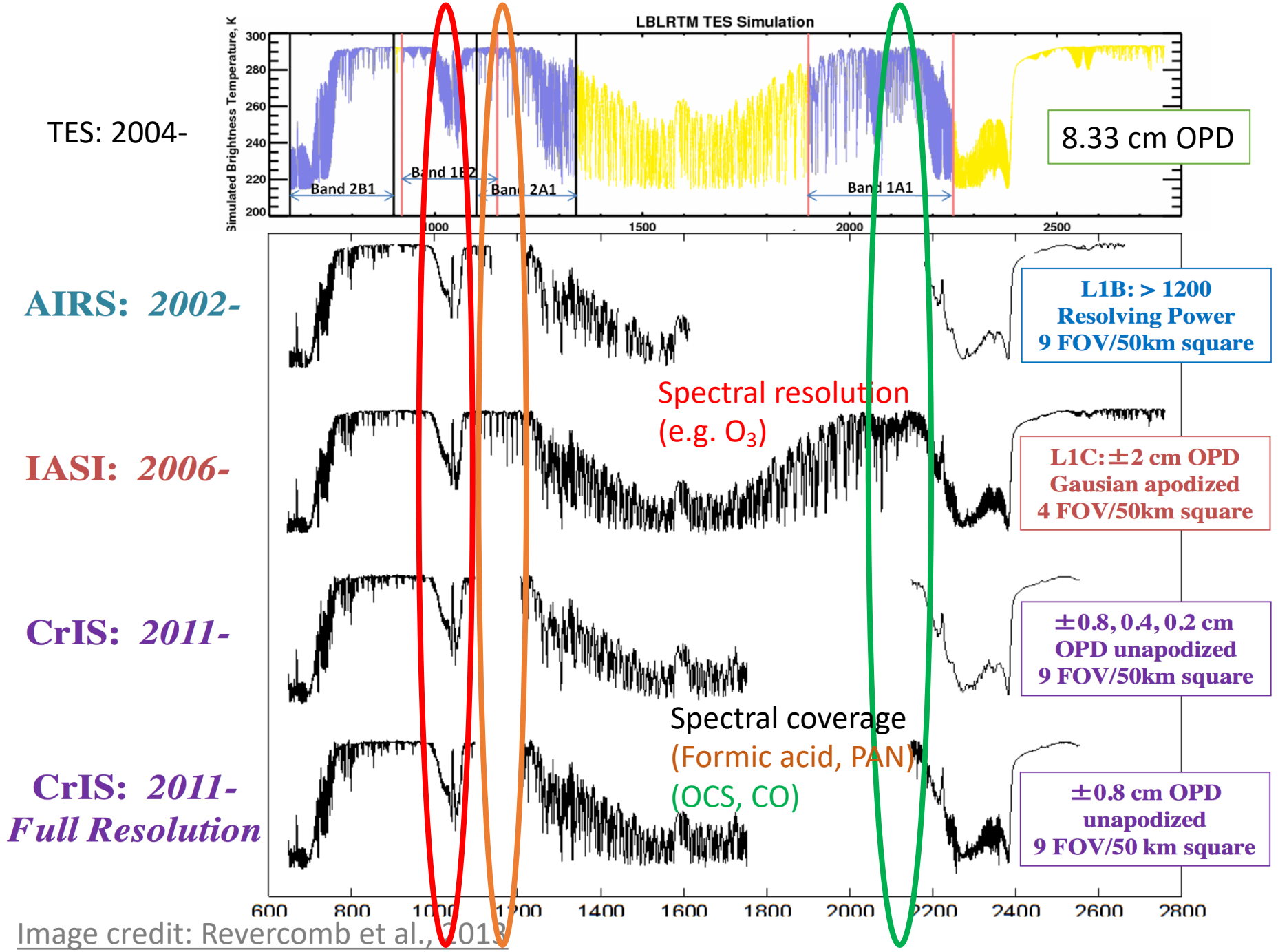
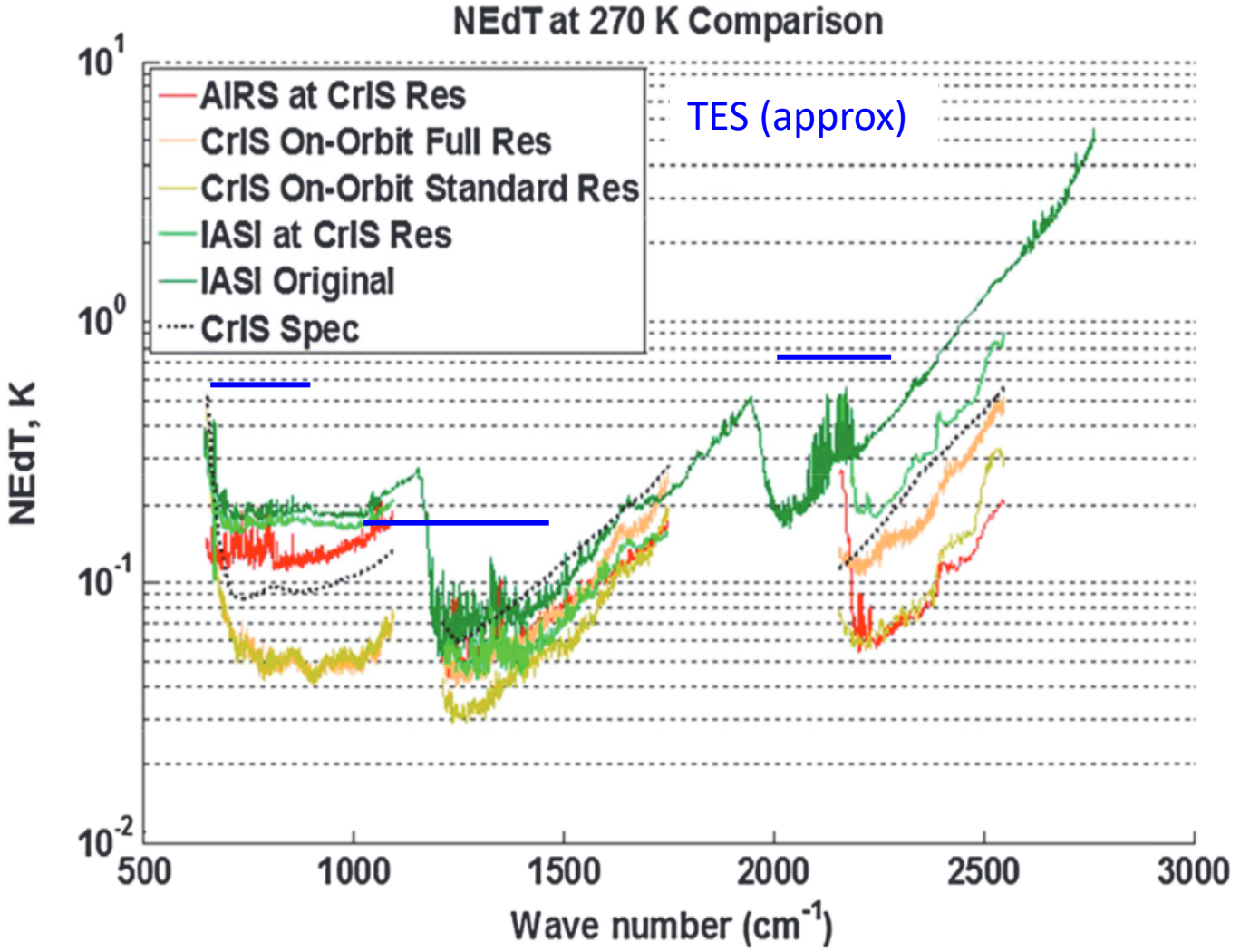


Image credit: Revercomb et al., 2013

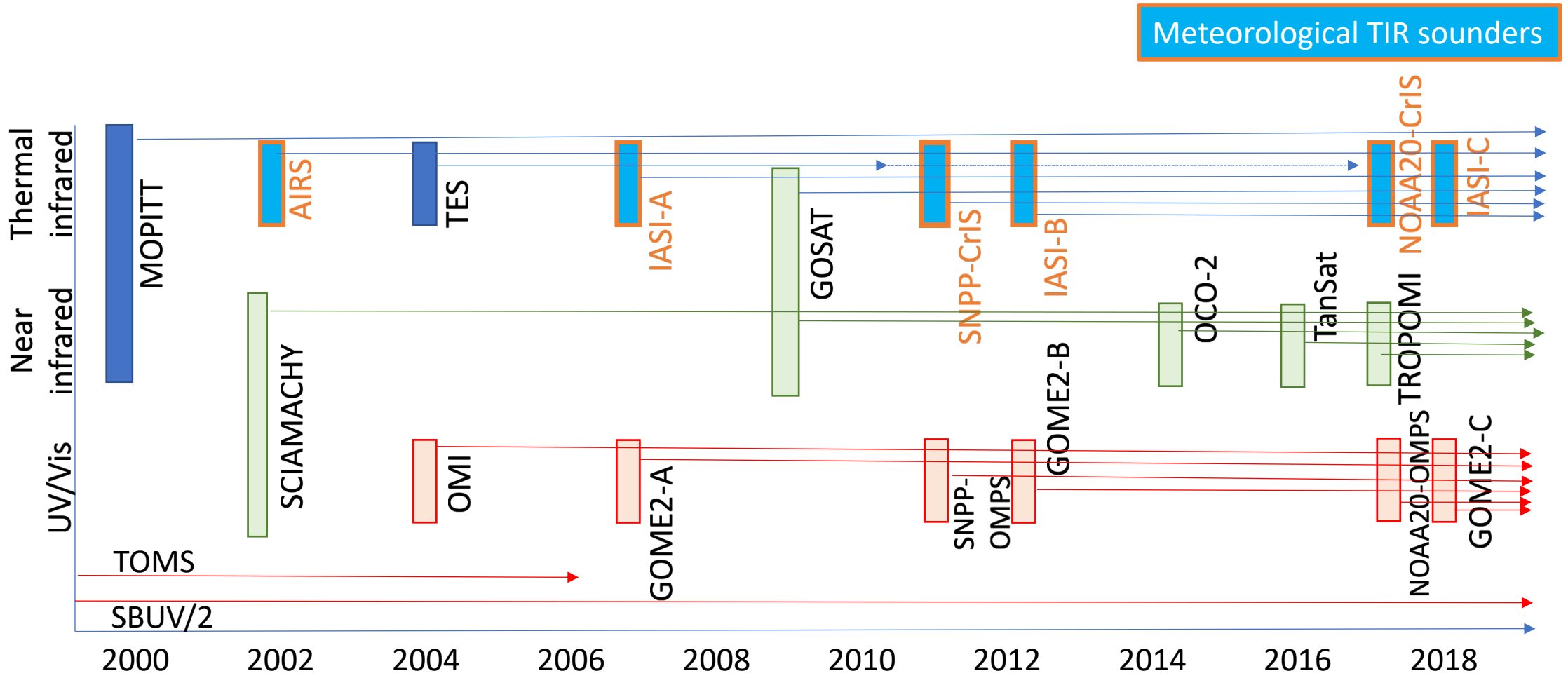
Instrument noise



CrIS Atmospheric Chemistry Data User's Report (September 2014)

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

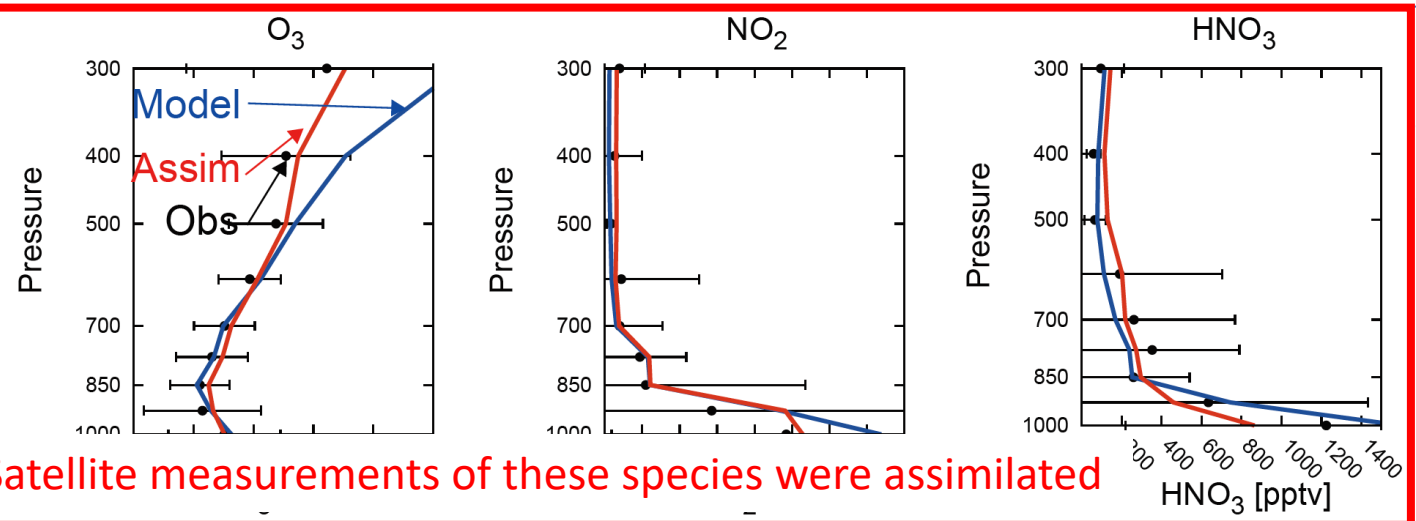
Nadir-viewing satellite measurements of composition in Low Earth Orbit



Chemical data assimilation

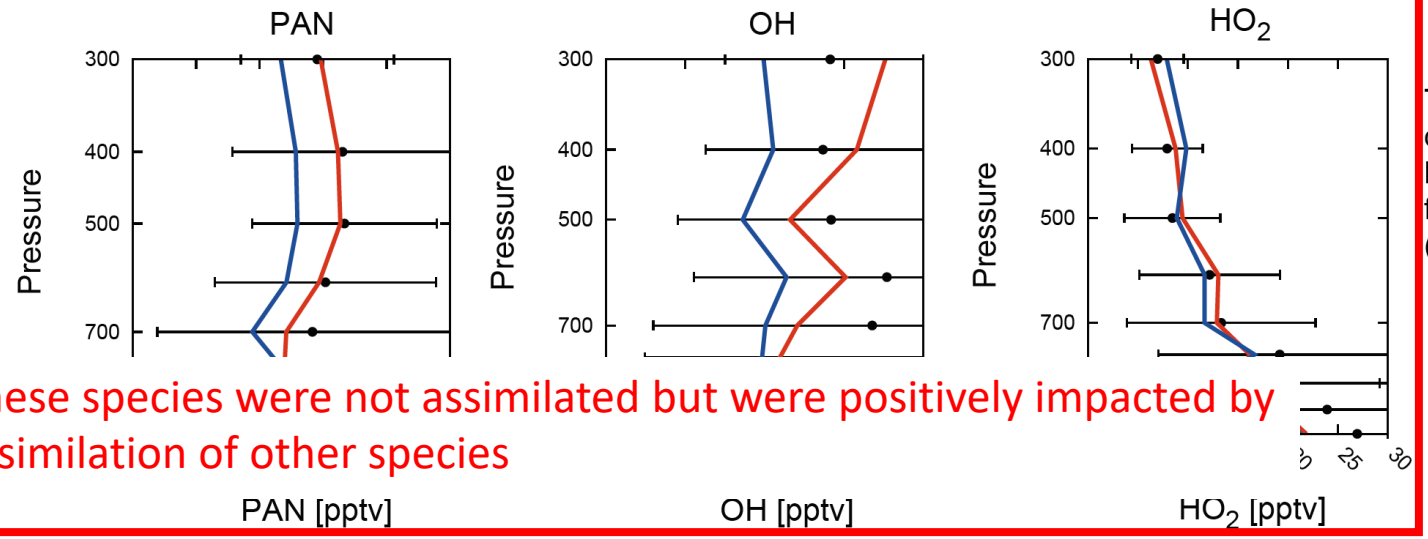
- Data assimilation for air quality forecasting

Chemical data assimilation:
Constraints on a range of species in the model



Satellite measurements of these species were assimilated

Fresh Canadian fire plumes were filtered out based on Simpson et al. (2011), because the fresh fire plumes can not be resolved at 0.56° resolution.



These species were not assimilated but were positively impacted by assimilation of other species

The 1-min merged observation data wereobtained from NASA LaRC Airborne Science Data for Atmospheric Composition (http://www-air.larc.nasa.gov).

- The data assimilation showed better agreements in assimilated (O_3, NO_2, HNO_3) and non-assimilated species (PAN, OH, HO_2) with the aircraft observations than the model simulation.

Takashi Sekiya, Kazyuki Miyazaki et al.

Presentation from 2018 IGAC meeting

ARCTAS-B period

Settings of assimilation

Assimilation scheme	Ensemble Kalman filter, 32 and 64 members
Forecast model	CHASER V4.0 (Sekiya et al., 2018) 92 species & 262 reactions
State vector	NO_x, CO, and SO_2 emissions, lightning NO_x, 35 chemical species
A priori emissions	HTAP_v2.2 (anth.), GFED4s (BB), GEIA (soil)
Period	Boreal summer (Jun. 22-Jul. 21) 2008
Resolution	Horizontal: 2.8, 1.1, and **0.56°** Vertical: 32 layers (to 4 hPa)

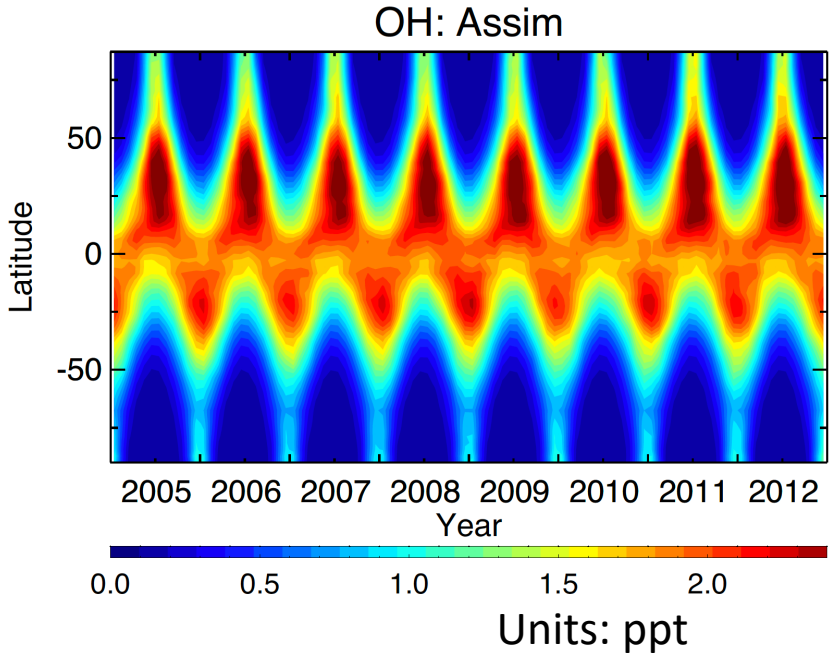
Assimilated observations

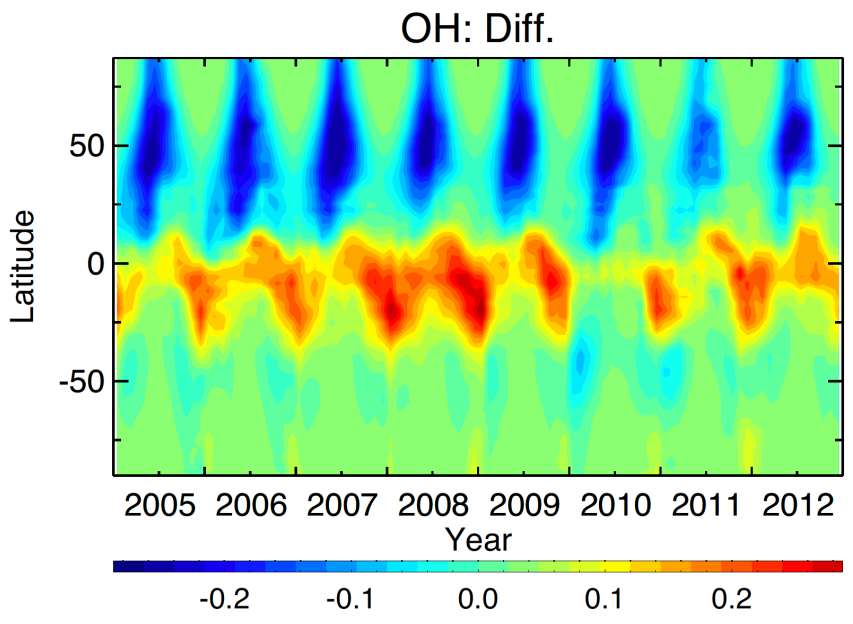
OMI, GOME-2, SCIAMACHY QA4ECV v1.1 Trop. NO_2 column	Boersma et al. (2017)
TES v7 O_3 profile	Herman and Kulawik (2013)
MLS v4.2 O_3 and HNO_3 profiles	Livesey et al. (2011)
MOPITT v7 NIR/TIR CO column	Deeter et al. (2017)
OMI v3 PCA SO_2 PBL column	Li et al. (2013)

Chemical data assimilation: Chemical reanalysis

- Example: Constraints on hydroxyl radical (OH) **[Miyazaki et al., 2015]**
  - "Detergent of the atmosphere"
  - Plays a key role in determining lifetime of other species
    - Impact on, e.g. CO trends, CH_4 growth rate….
  - Extremely challenging to measure
    - Currently no way of measuring tropospheric OH directly from space, but multi-species assimilation can provide constraints on model OH

Assimilation of:
OMI NO_2
TES O_3
MLS O_3 and HNO_3
MOPITT CO





Evaluation of products

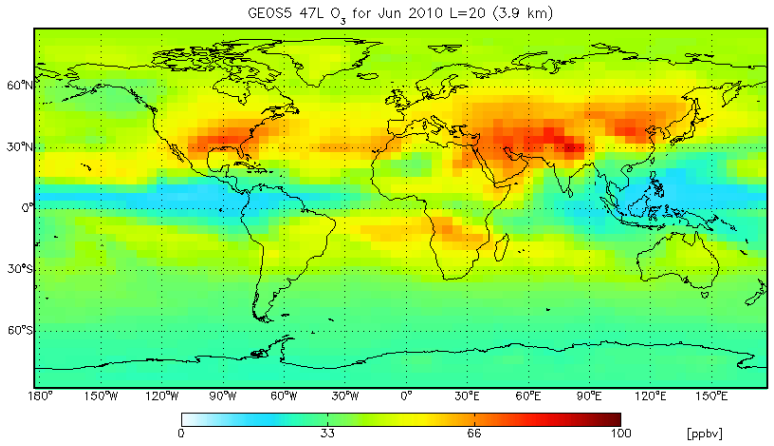
- Basic testing
  - Information on processing time
  - Sanity check
    - Do we see expected global/seasonal variation?
    - Do we see any obvious pronblems? (Scan angle dependence, etc.)
    - Summary of info on vertical information
  - Evaluate bias and rms with respect to reference datasets
  - Comparison of estimated vs actual errors
  - Basic check on time dependence of bias
  - Basic check on time dependence of error estimates

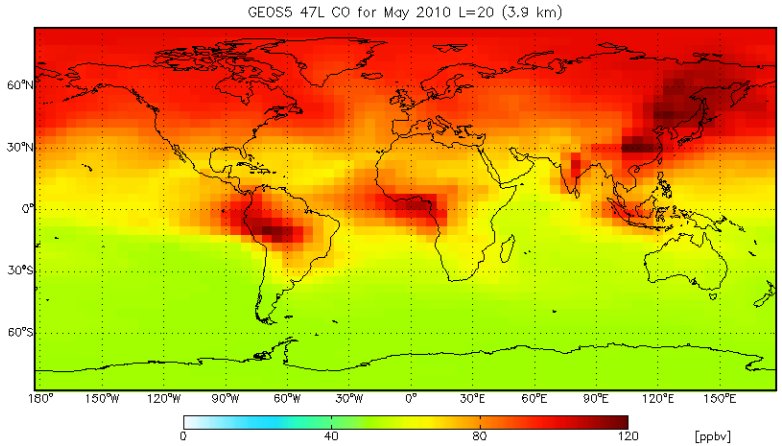
- Extended testing?
  - Evaluation of continuous time series relative to reference datasets
  - Evaluation of suitability of dataset for particular science questions

Evaluation of composition products: Quick Test Sets

- **”Quick test sets”** for each molecule, instrument
  - Different types of potential test sets:
    - Sanity checks / characterization of vertical information content by location/season
    - Characterization of biases and error estimates with respect to reference measurements
    - Characterization of changes in time
  - Evaluate the characteristics of any given product
    - Summary of product characteristics for a given algorithm/instrument
      - **Key information for users!**
    - Evaluate algorithm updates
  - **~50,000 – few 100,000 cases per set**

Sanity check





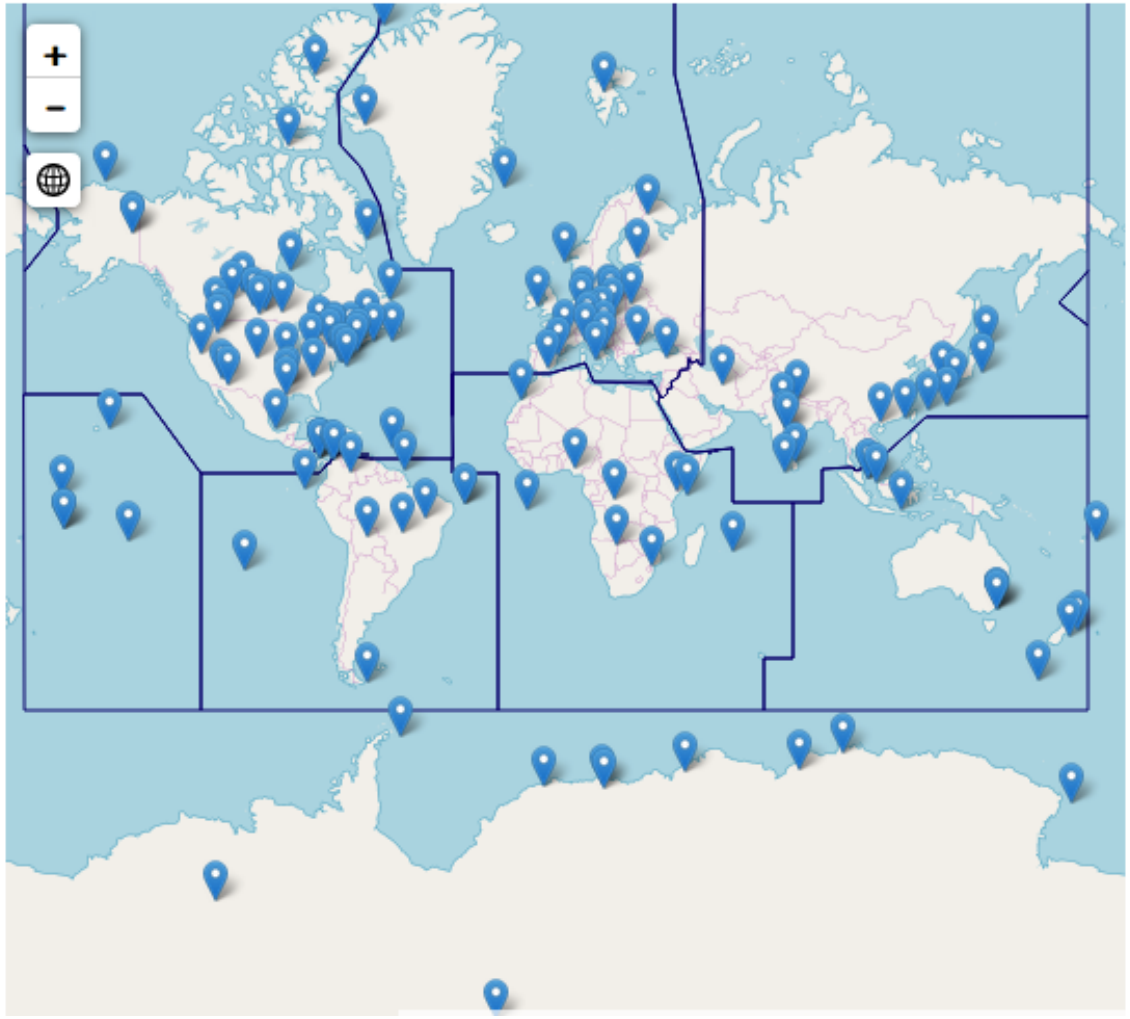
- 8 months of data being used for algorithm evaluation at Sounder SIPS
  - January/April/July/October 2013, 2015
  - Covers different seasons, different years
- Subset of this would be sufficient for sanity check
  - 1 month of data at TES-like nadir sampling: ~50,000 cases
  - Sub-sampled set from these 8 months could
    - show global distribution, enable evaluation of vertical information over range of conditions

Comparisons with reference datasets

- For characterization of bias, rms and estimated vs actual errors, we ideally want a dataset of independent reference profiles that
  - Cover the vertical range over which the satellite retrievals are sensitive
  - Span a range of atmospheric conditions
    - Temperature, humidity, vmr profiles
    - Cloud(?)
  - Span a range of surface conditions

  - Cover a long time period (maybe “extended” testing?)

Ozone: WOUDC ozonesondes



World Ozone and Ultraviolet Radiation Data Center

Vertical profiles of ozone starting in 1951

Ozonesonde comparisons: coincidence criteria

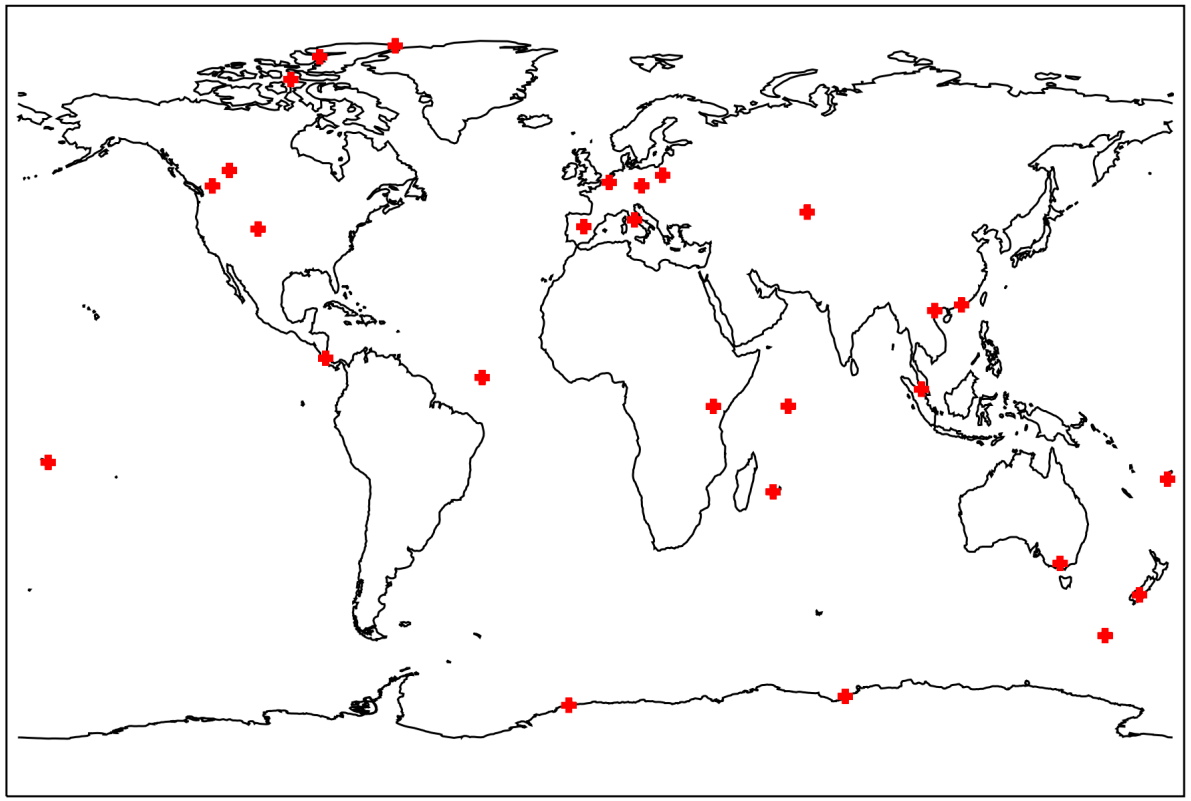
Considerations: Spatial scales of atmospheric variability for the species vs number of profiles available for validation

Document	Instrument(s)	Radiance input	Time criteria	Spatial criteria	Time period
Divakarla et al. [2008]	Aqua-AIRS	L2 cloud-cleared	-3h < dt < +3h	< 100 km	2002-2005
			-12h < dt < +12h		
Nalli et al. [2018]	SNPP-CrIS	L2 cloud-cleared	-4h < dt < +2h	< 125 km	2012-2015
Dufuor et al. [2012]	MetOp-A IASI	L1C	-7h < dt < +7h	< 110 km	2008
Oetjen et al. [2014]	MetOp-A IASI	L1C	-7h < dt < +7h	< 110 km	2008
Boynard et al. [2016]	MetOp-A and MetOp-B IASI	L1C	-10h < dt < +10h	< 50 km	2008-2014
TES v7 validation report	Aura-TES	L1B	-9h < dt < +9 h	< 300 km	2006-2009
Fu et al. [2018]	AIRS/OMI	L1B	-4h < dt < +4 h	< 300 km	2006

AIRS FOV match-ups, subset of WOUDC sites

- Coincidence criteria:
  - t < 4 h, distance < 200 km

- Jan 2015: 20529 matches
- April 2015: 23611 matches
- July 2015: 19708 matches
- Oct 2015: 16950 matches



Precision of the retrievals (ozone examples)

- Keim et al. 2009
- Dufuor et al 2012

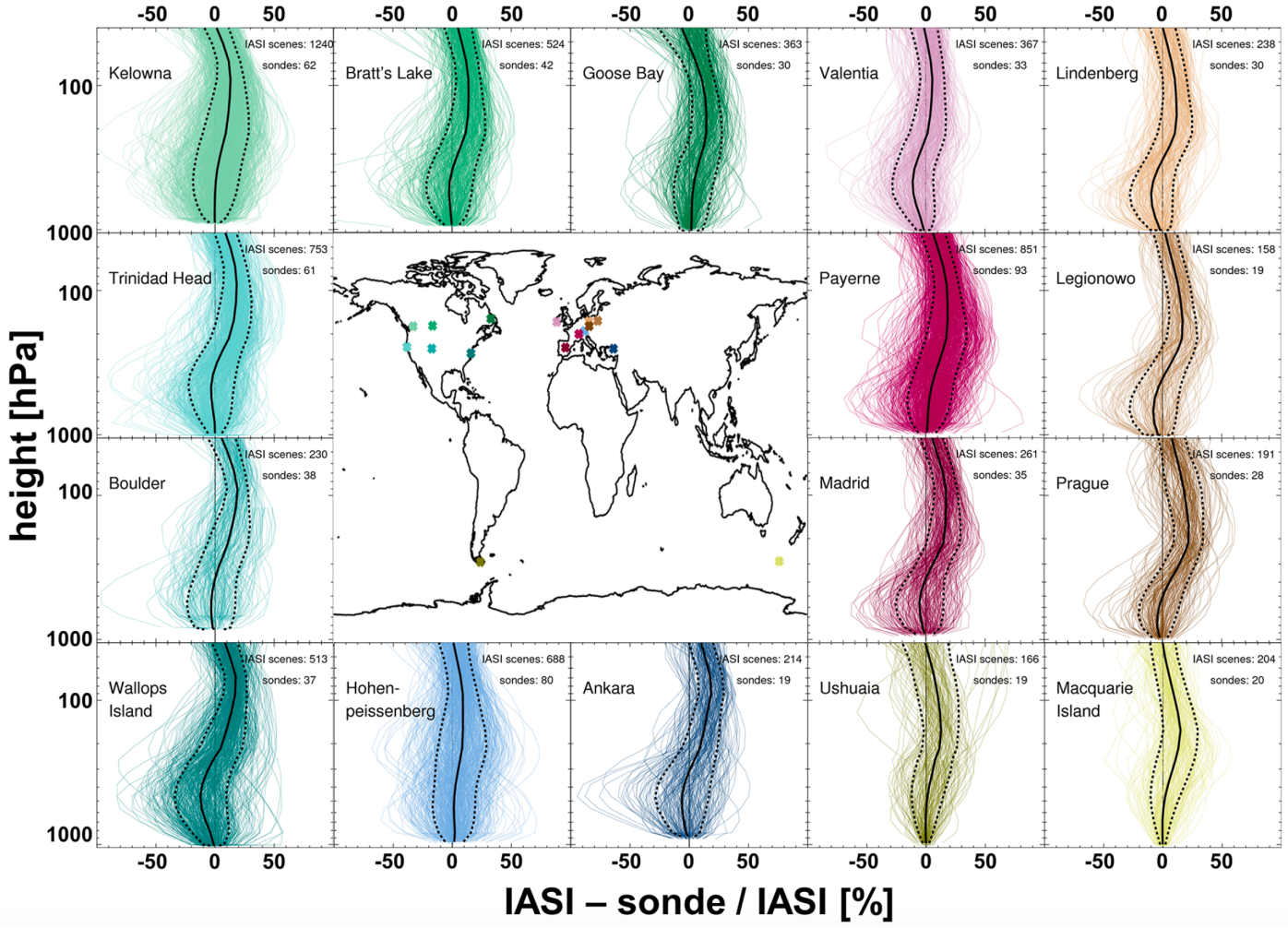
→ Compare random error estimate from the retrieval to the rms of the difference between the retrieved and the smoothed sondes

- Boxe et al.
- Oetjen et al. 2014

→ Covariance approach, accounting for random (noise) error, temperature and water vapor error propagation.

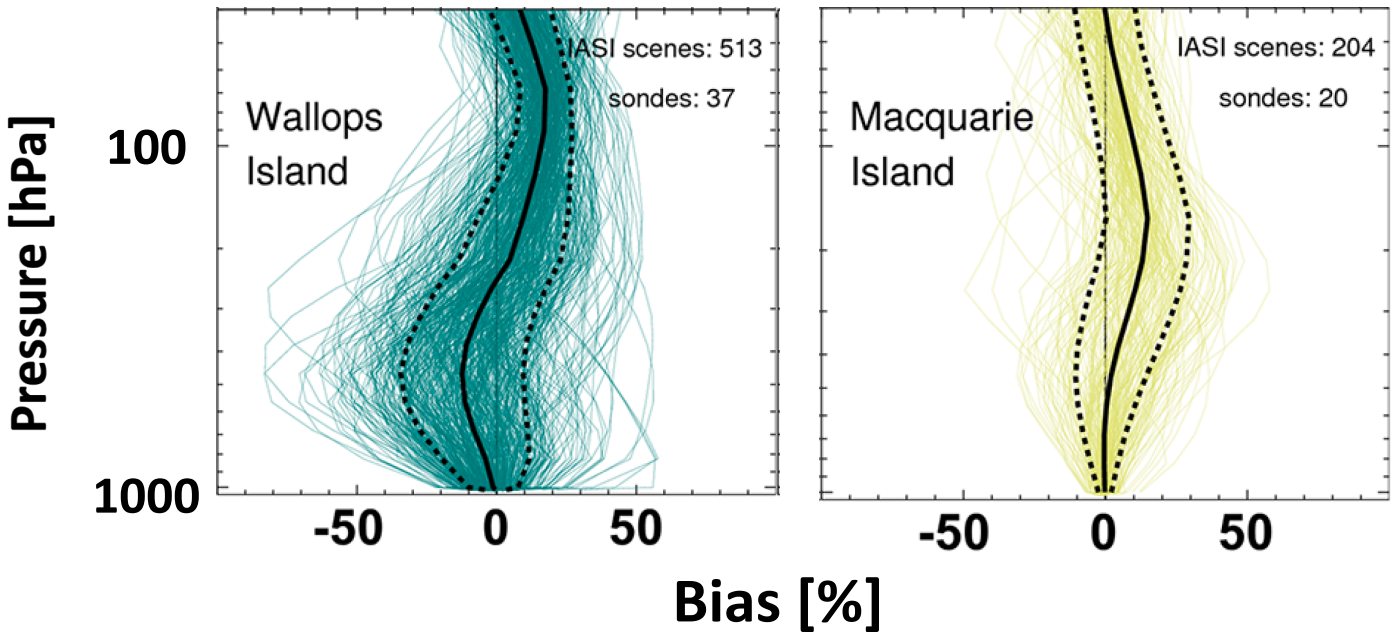
Examples of sonde comparisons (IASI)

Observation operator applied to sonde profiles for comparisons

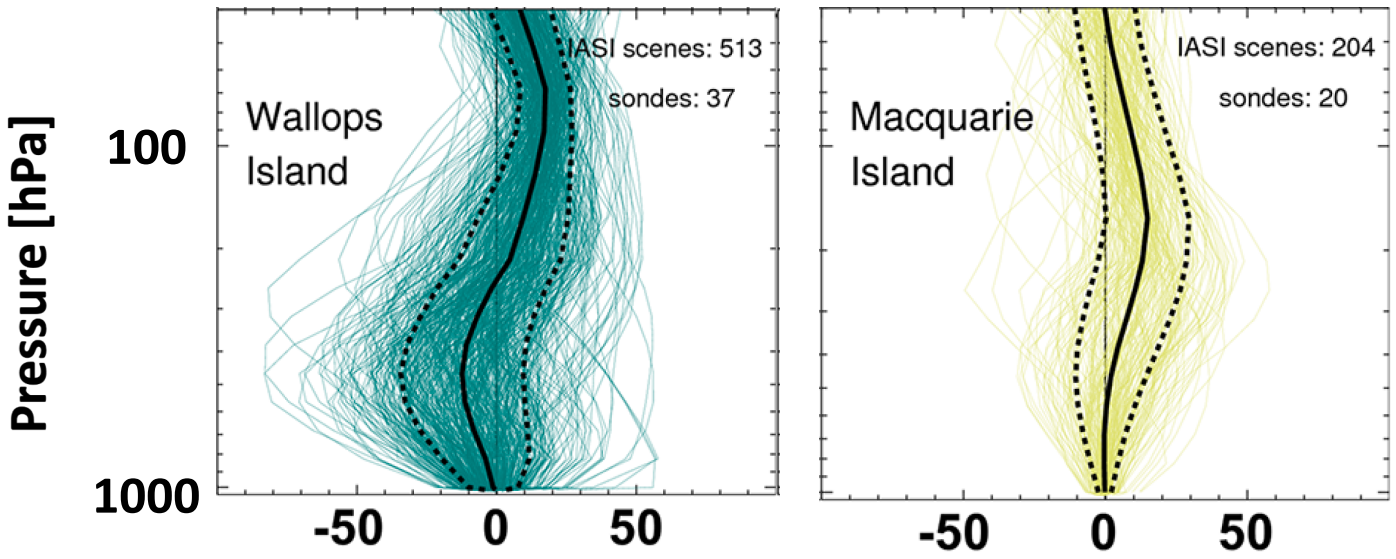


Oetjen et al., [2014]

Estimated vs actual error



Estimated vs actual error



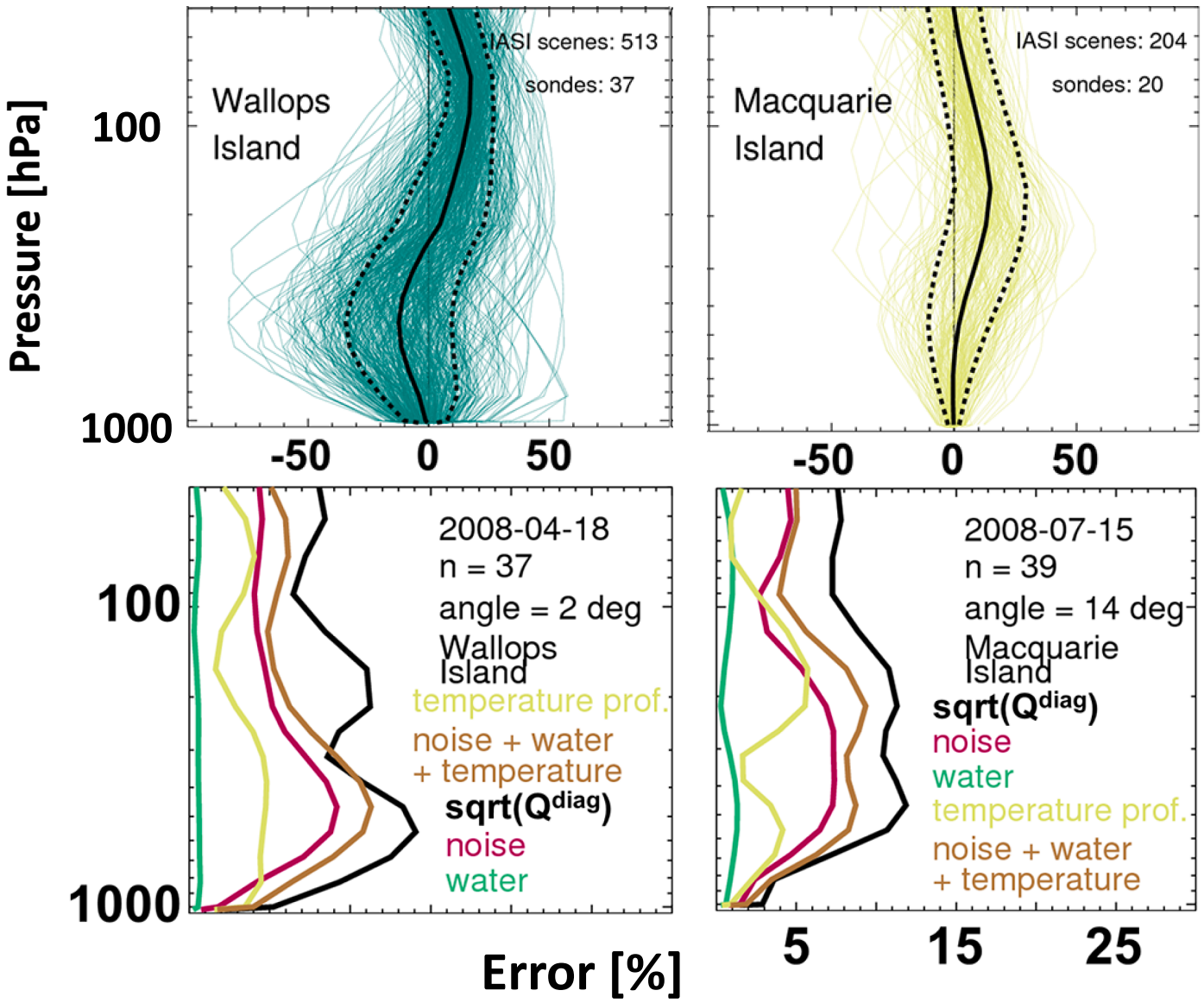
Sample error covariance:

Assume O_3 does not vary.

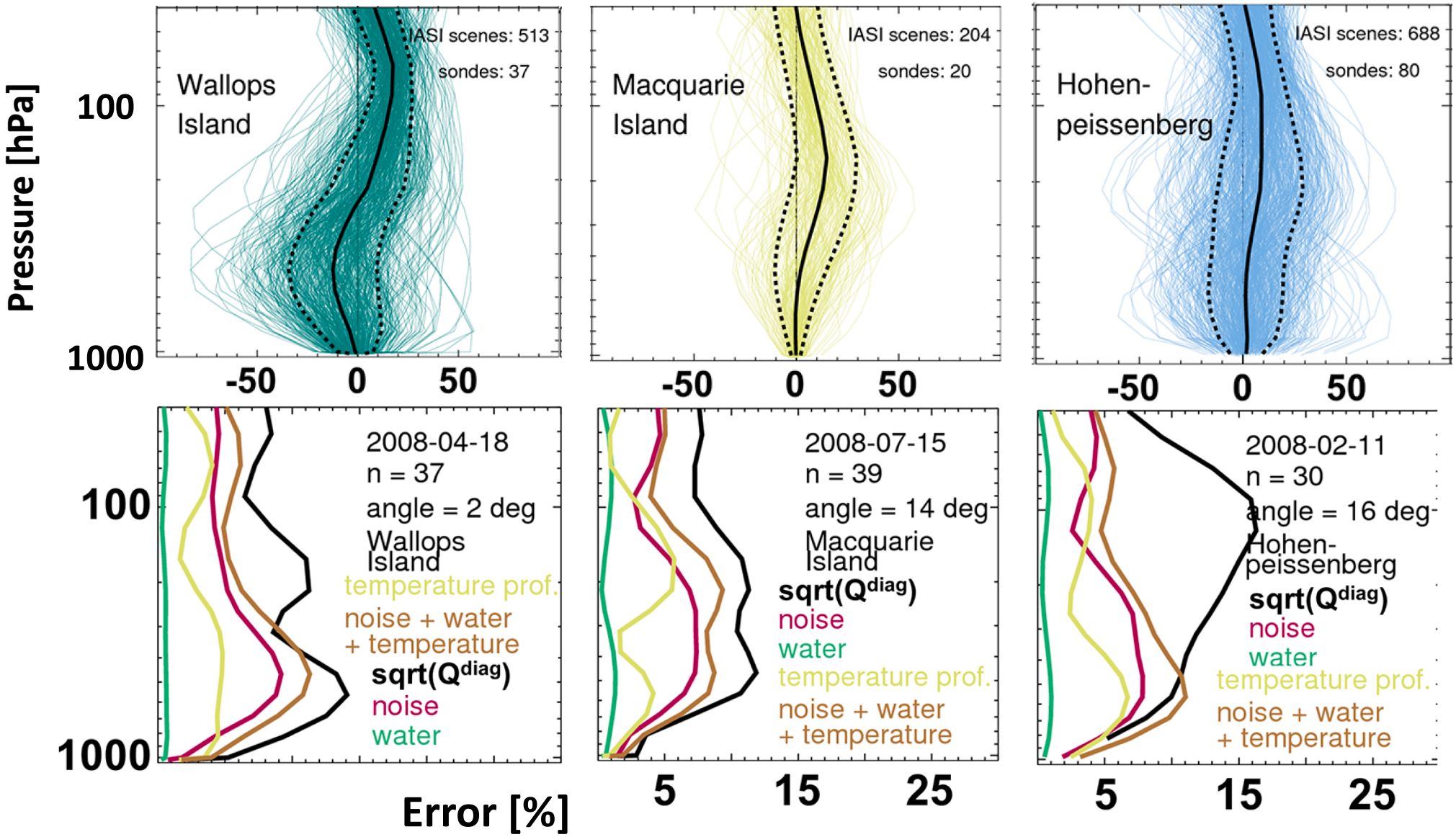
IASI FOVs within 100 km radius, same IASI granule

$$\mathbf{Q} = \frac{1}{n-1} \sum_{i=1}^{n} \left(z_i - \bar{z}\right) \left(z_i - \bar{z}\right)^{\mathsf{T}}$$

Estimated vs actual error



Estimated vs actual error



Aircraft campaigns: HIPPO and ATom

- HIPPO campaigns:
  - Jan 2009
  - Oct - Nov 2009
  - Mar – Apr 2010
  - Jun – Jul 2011
  - Aug – Sept 2011

- ATom campaigns:
  - Jul– Aug 2016
  - Jan – Feb 2017
  - Aug – Sep 2017
  - Mar – Apr 2018

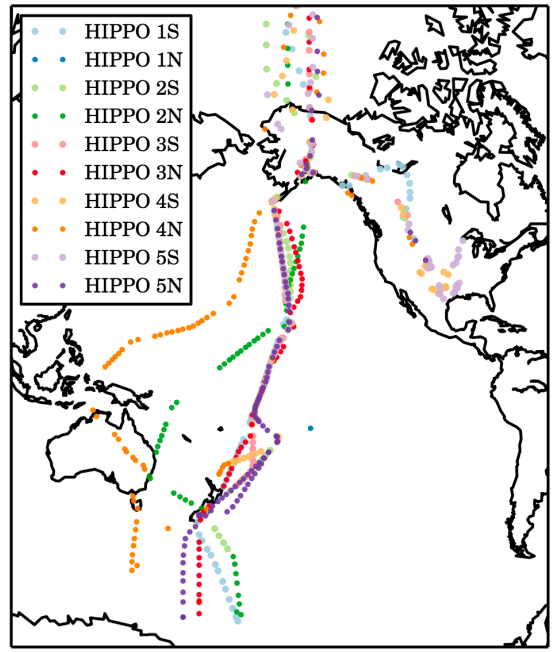


Figure: Frankenberg et al. [2016]

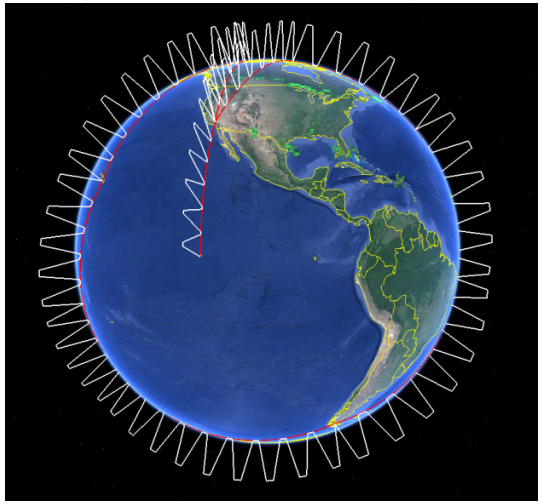


Image: https://espo.nasa.gov/atom

Aircraft campaigns: HIPPO and ATom

- HIPPO: Already been used extensively for satellite validation
  - CO_2, CH_4, CO, N_2O
- ATom profiles provide an additional reference dataset
- Vertical extent:
  - Up to 14 km for select cases
  - Need to make some assumption above top of measured profiles
  - Most useful for species where most of column amount lies in troposphere
- Most profiles are over remote ocean
- Coincidence criteria: Species-dependent
- Example: +/-9 hours, 50 km for CH_4 (S. Kulawik)
  - Results in 23,059 AIRS FOV matches for all 5 HIPPO deployments

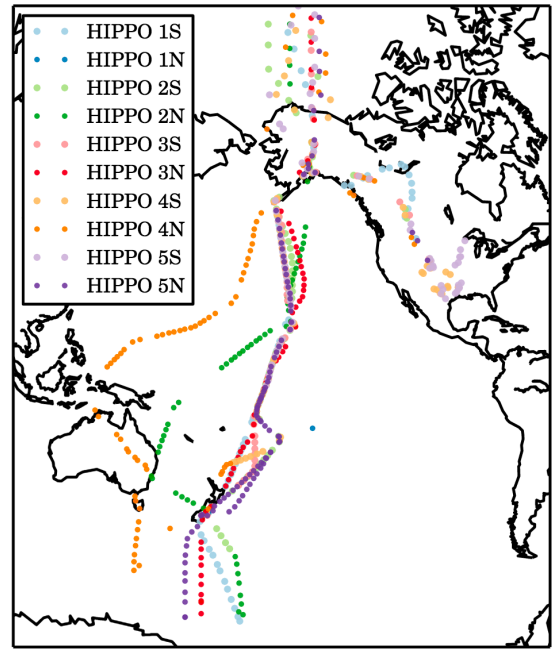


Figure: Frankenberg et al. [2016]

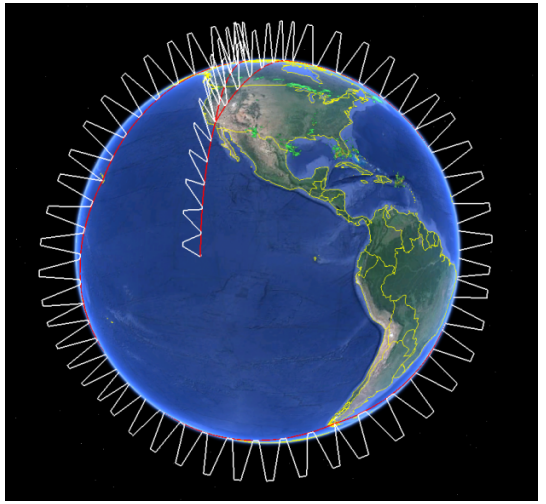


Image: https://espo.nasa.gov/atom

Summary

- Characterization of vertical sensitivity (averaging kernels) and **error estimates** are key to maximizing the scientific utility of the sounder composition products.

- Validation of error estimates ought to be part of algorithm/product evaluation.

Goals

- Establish species- and instrument-dependent “quick test sets” for:
  - Sanity checks
  - Evaluation of differences in sensitivity diagnostics
    - between algorithms or algorithm versions
  - Evaluation of bias, rms with respect to reference datasets
  - Evaluation of estimated vs actual error
  - Initial assessment of changes over time (or lack thereof)

- For some molecules, we have datasets that can be readily utilized
- **Start with test sets based on**
  - **WOUDC ozonesondes (O_3)**
  - **HIPPO and ATom (CO, CH_4, CO_2)**
- For some other molecules, evaluation may be more challenging….

Backup slides

From AIRS v6 L2 product user guide

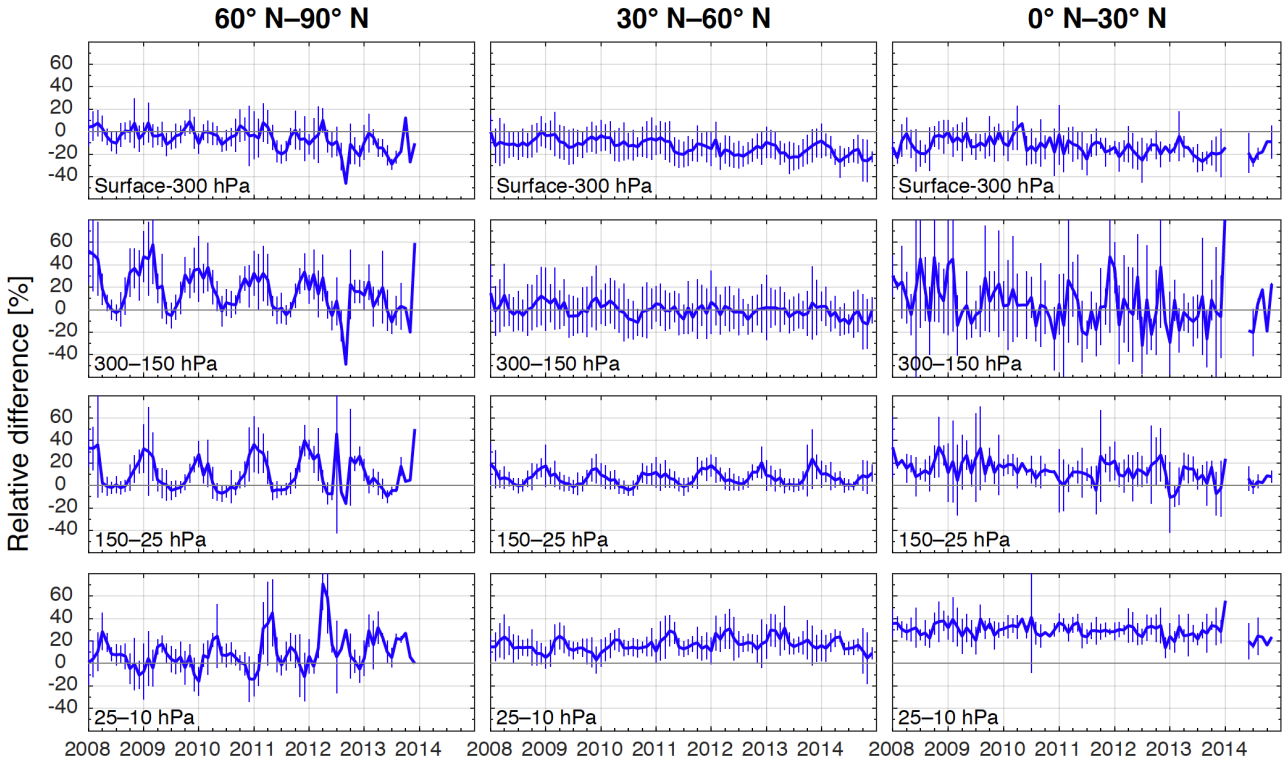
The error fields, including **O3VMRLevStdErr**, **O3VMRStdErr, O3VMRLevSupErr, O3CDSupErr** and **totO3StdErr**, are fixed as a fraction of the ozone amount and should not be used.

Variation in time: Ozone

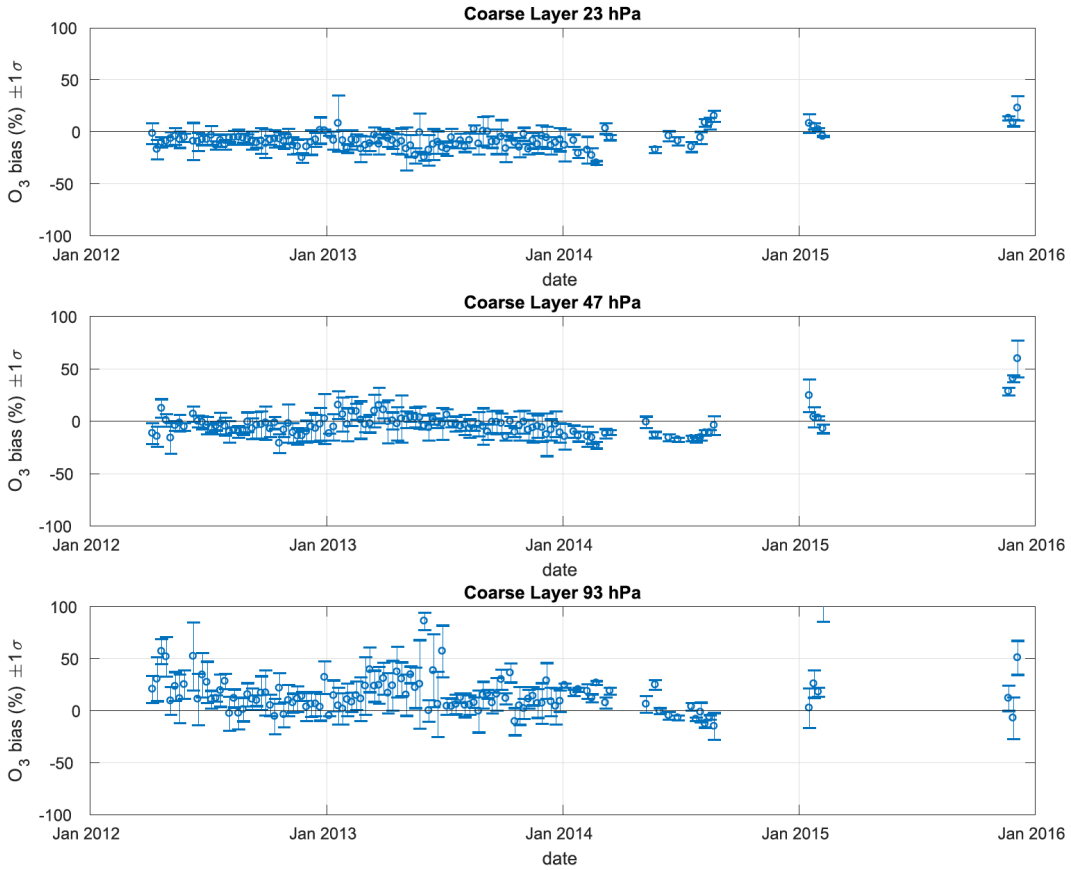
- Boynard et al. [2016]
- Nalli et al [2018]

Variation in time: Other molecules

- Aircraft campaigns provide snapshots in time
- For long-term records, look to ground-based networks



Boynard et al., 2016



Nalli et al., 2018

SNPP NUCAPS Cal/Val Ozonesonde Sites (2012-2015)

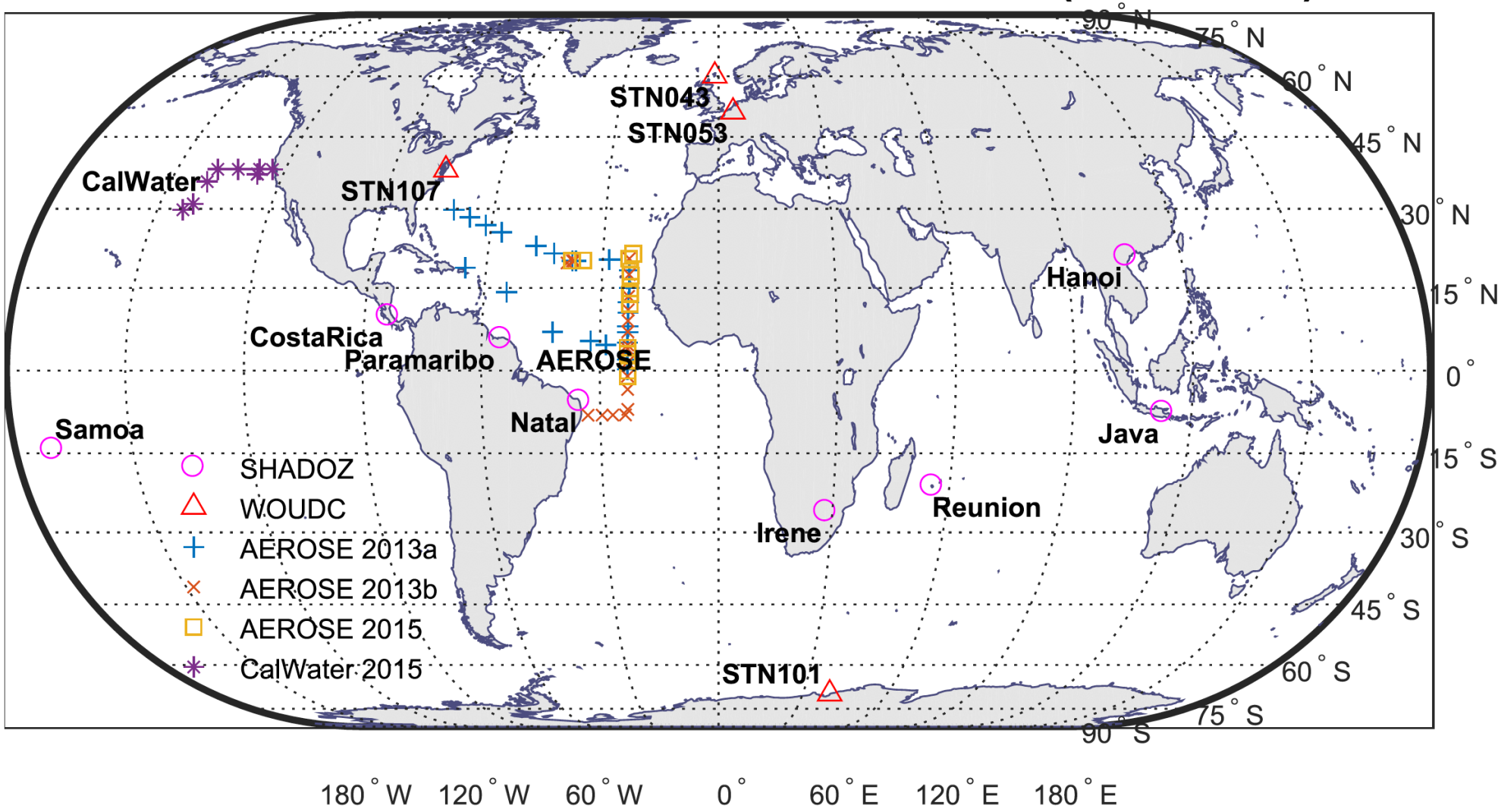


Figure: Nalli et al. [2018]. Ozonesonde truth sites used for SNPP NUCAPS IR ozone profile EDR cal/val over the sampling period 2012–2015.

Total Carbon Column Observing Network (TCCON)

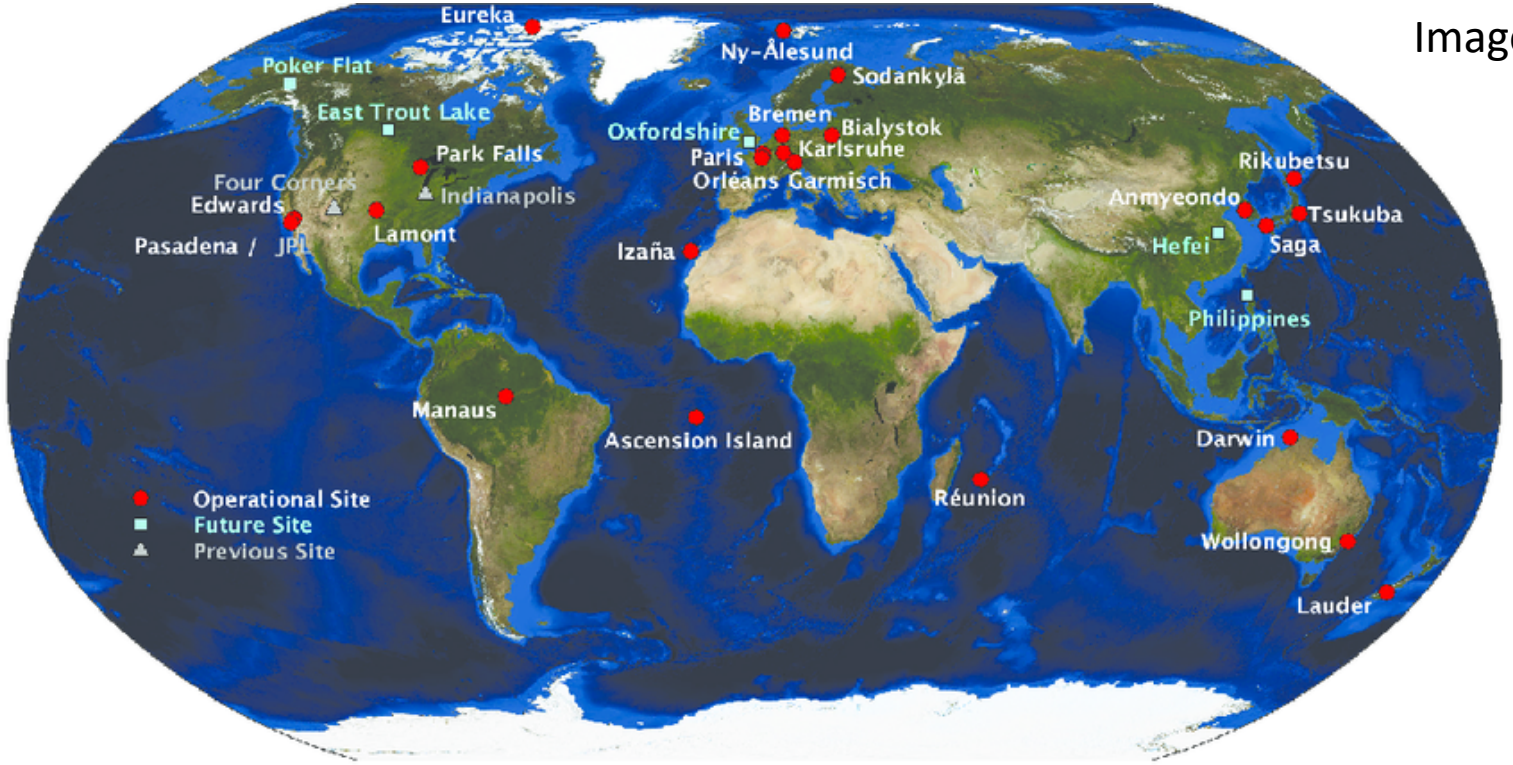
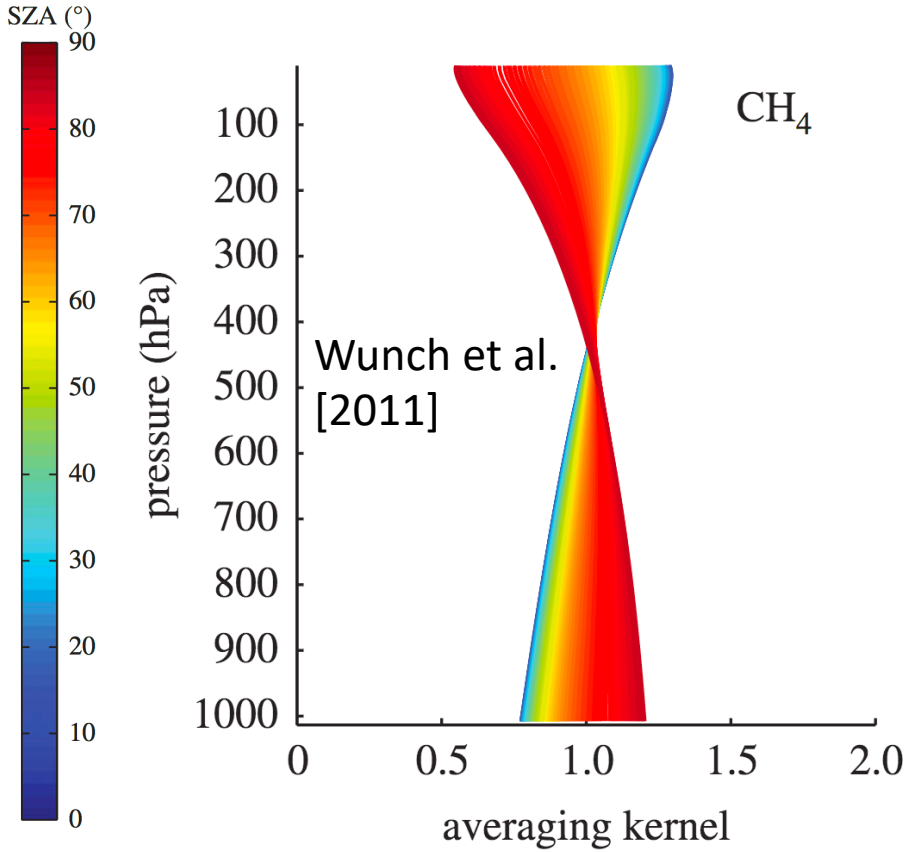


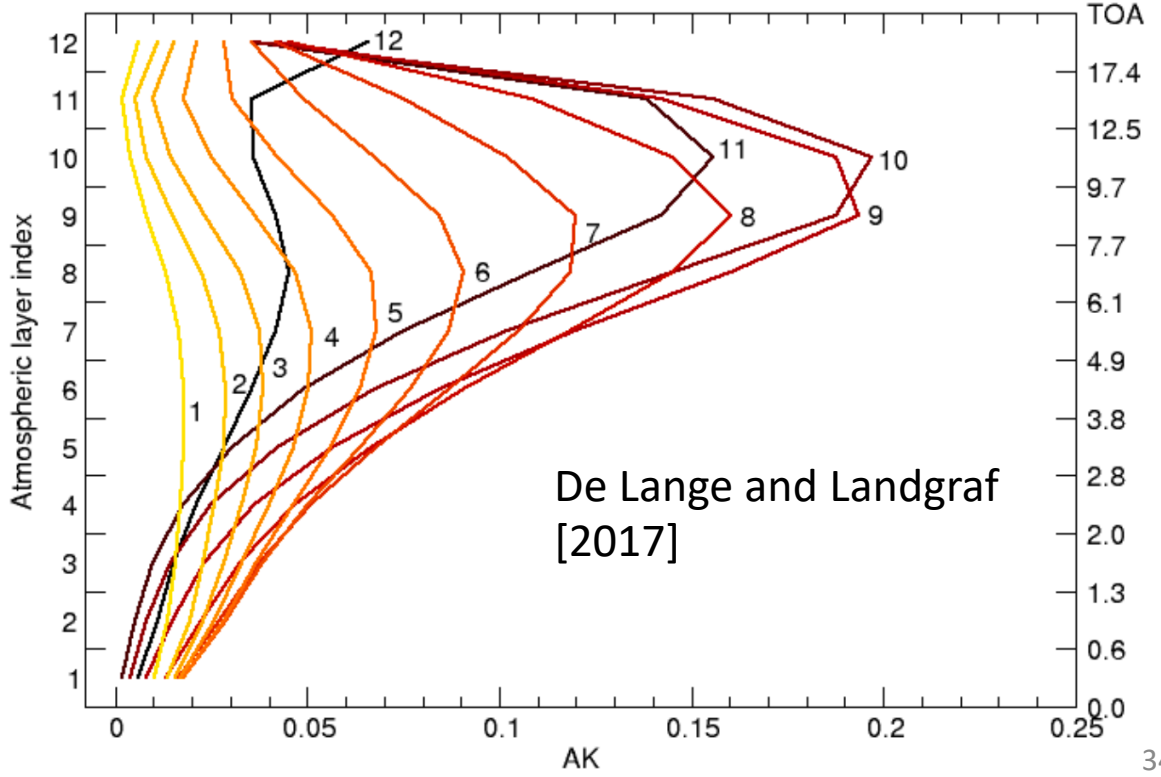
Image: Dupuy et al. [2016]

TCCON column-average products include XCO2, XHC4, XCO, XN2O, XH2O, XHDO

TCCON

- TCCON measurements are sensitive throughout the column
- IR sounders are <u>not</u>
  - Comparisons should account for differences in vertical sensitivity





Evaluation of time series with TCCON?

- TCCON retrievals: Retrieved quantity is column-average

- One possible approach: De Lange and Landgraf [2017]
  - Applied to validation of thermal IR retrievals of CH_4
  - Take chemistry transport model field
  - Assume reasonable model profile shape
  - Scale model profile by TCCON column-average
  - Apply IR averaging kernel and prior to scaled model profile
  - Compare
- Works if variability in column-average is driven by variability in vertical range where satellite retrievals are sensitive

Network for the Detection of Atmospheric Composition Change