A review of Tropospheric O_3 observation from space: infrared sounding

Introduction
- I. Background of O_3
- II. Review of infrared sounders

Methodology
- III. Intercomparison of sensors and models
- IV. Trop. O_3 retrieval of GOSAT

Conclusion
- V. Research plan

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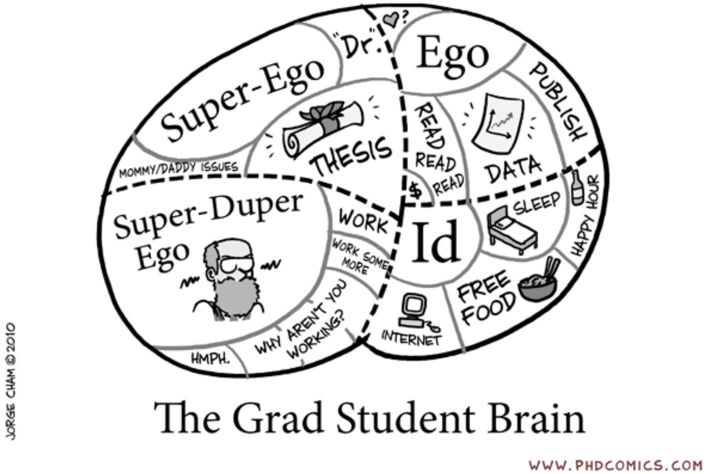
Collaborator: Dr. Paul T. Griffiths



Introduction

The climatic property and mechanism of Ozone (O_3)

- O_3 is <u>secondary pollutant</u>
  - Chapman cycle in stratosphere
  - VOC + NO_x + CO cycle in troposphere
  - Sensitive to [HO_x], [NO_x], sunlight in trop.

  Major sink *Major source* *Affect rate coefficient*

- O_3 is <u>short-lived climate forcer (SLCF)</u>
  - Lifetime ~ hours to weeks (depends on latitude) → 19 days in avg.

$PO_3 \propto [H_2O]$ & sunlight

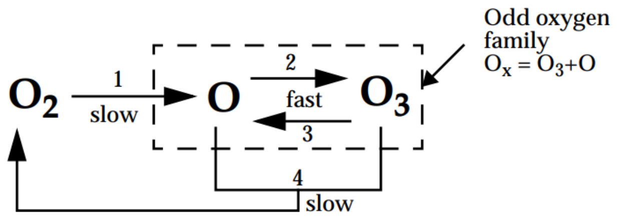
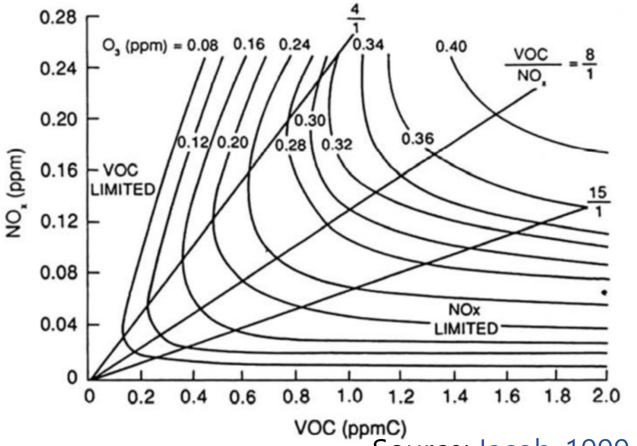
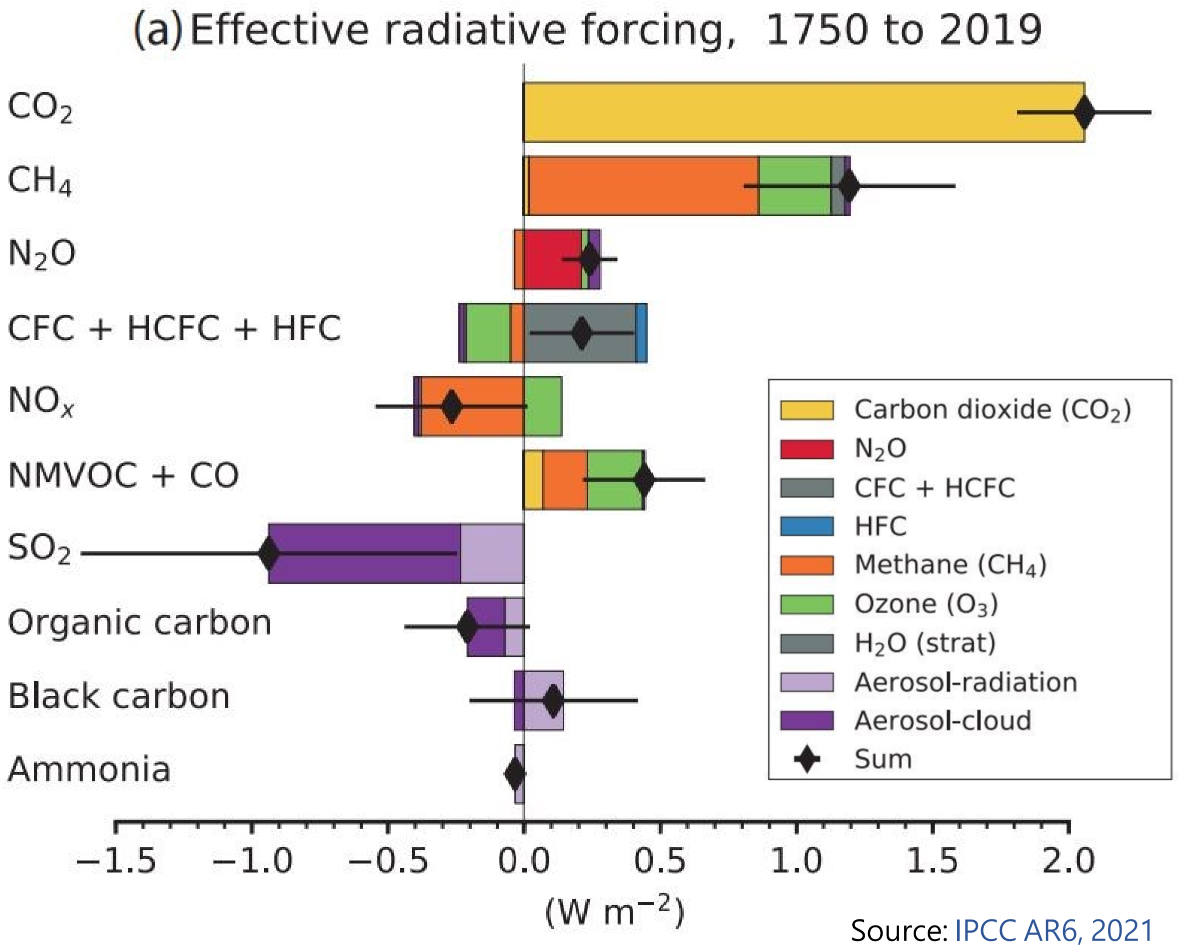


Figure 10-3 The Chapman mechanism

Source: Jacob, 1999



Source: Jacob, 1999

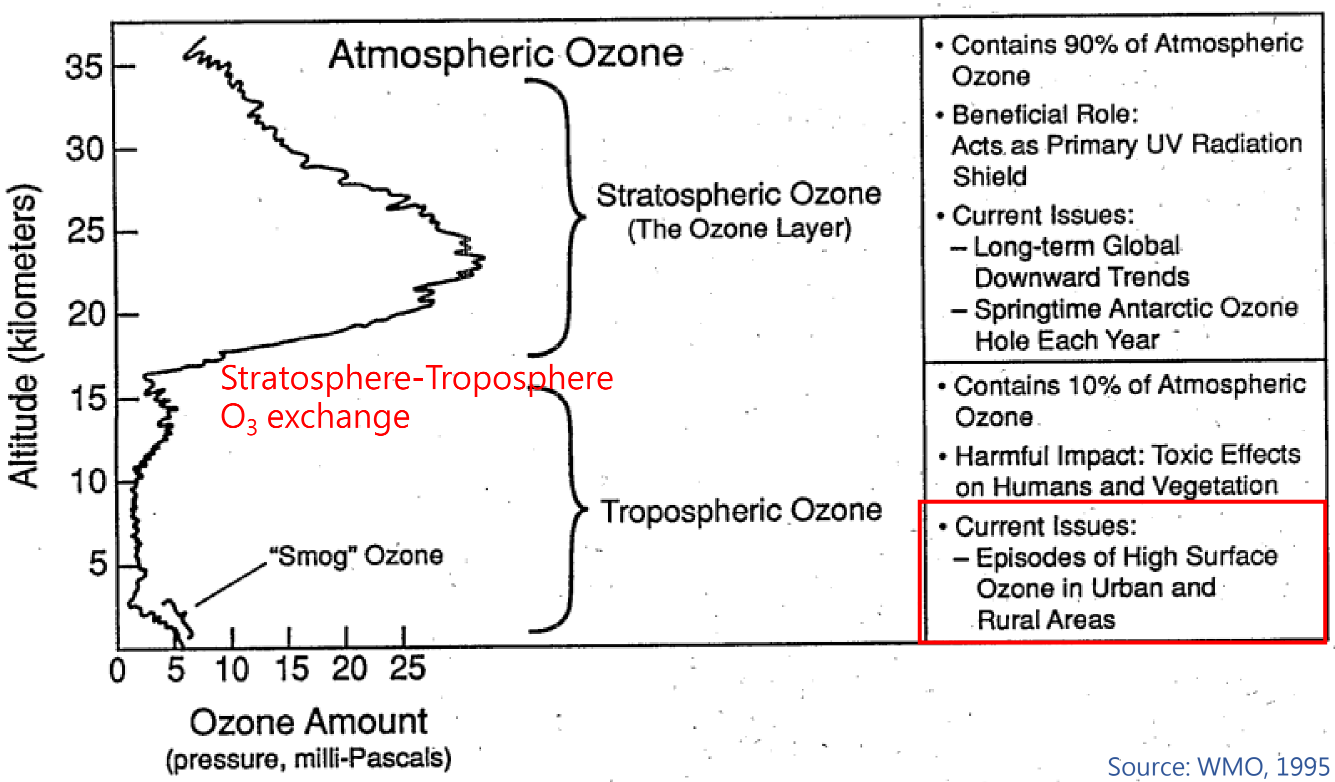


Source: IPCC AR6, 2021

Introduction

A typical vertical profile of Ozone (O_3)

- Ozone layer at 15~30 km
  - Absorb UV light (200-340 nm)
  - Ozone hole over South Pole
- Stratosphere-troposphere exchange at 10~15 km
  - Brewer-Dobson circulation (over the tropics)
- Surface "smog" < 3 km
  - Smoke + frog = smog
  - Product of NOx and VOC
  - "Great Smog of London" (1952)



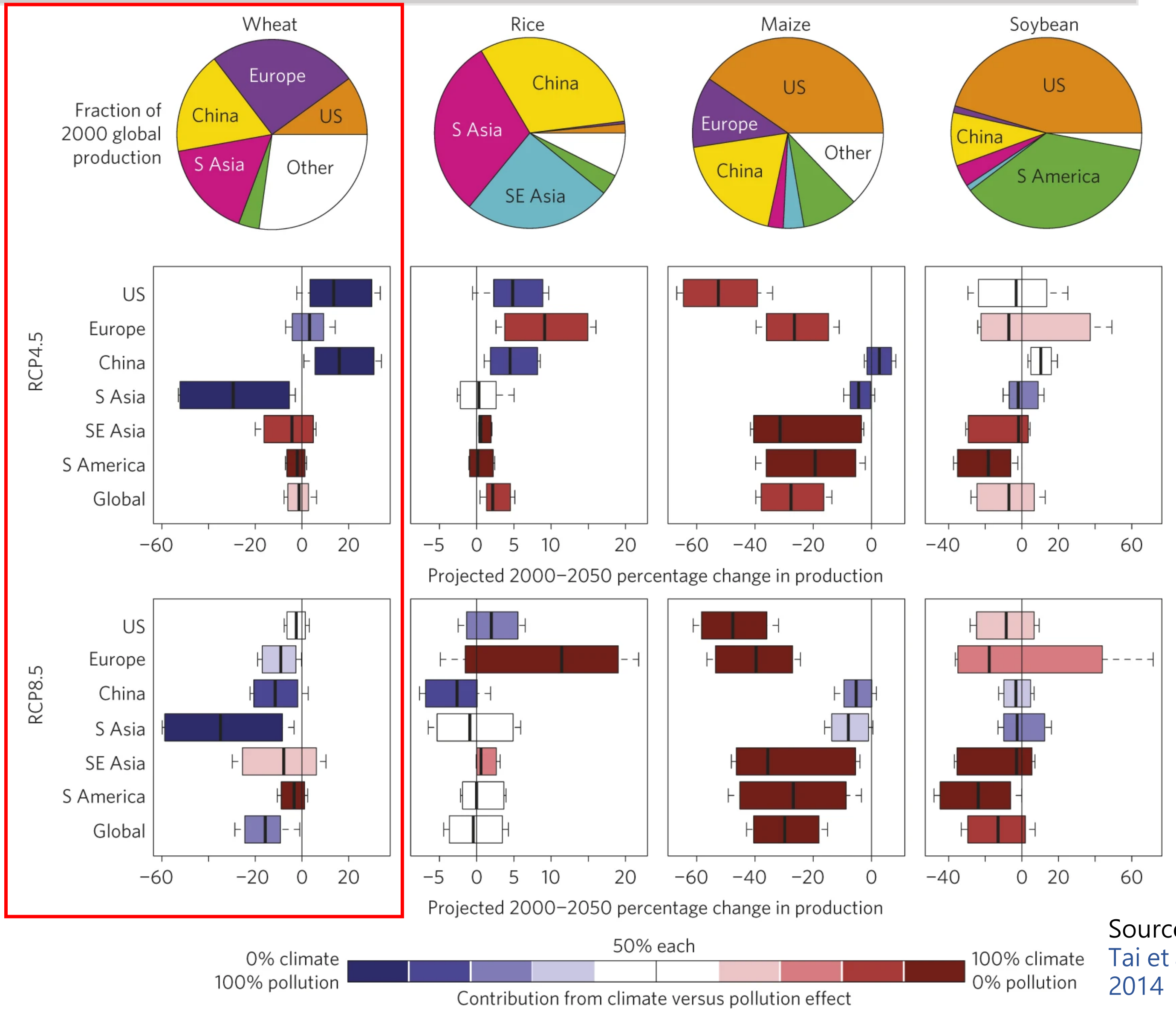
Source: WMO, 1995

Introduction

The impacts of Ozone (O_3): health and food

- Surface O_3 smog
  - ! Ignites respiratory tract
  - ! Crop production (esp. wheat)
- O_3 damage vs heat damage
  - Regional
  - Categorical
- For example
  - Climate change: Maize, Soybean
  - O_3 pollution: Wheat

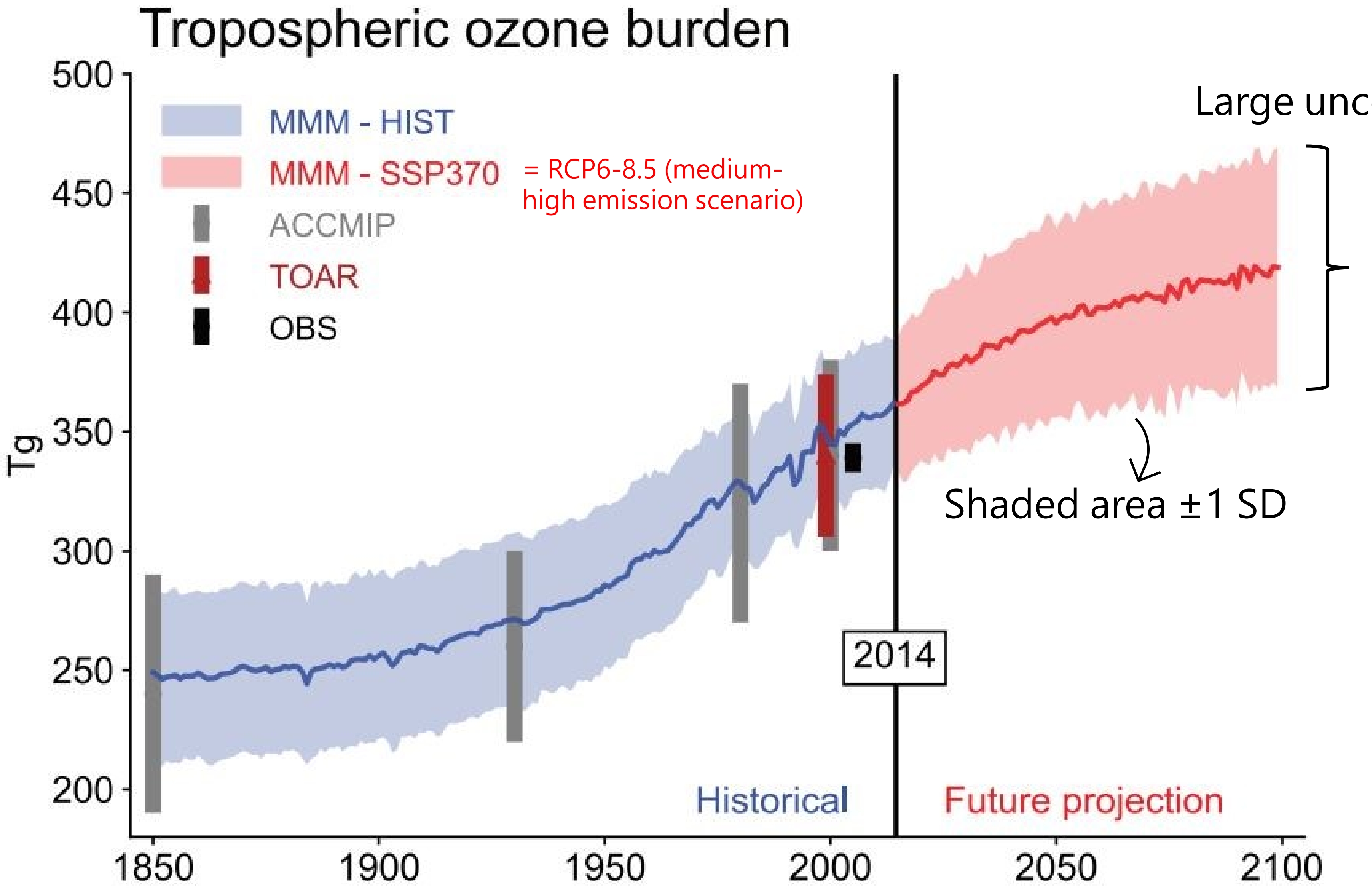
∴ O_3 does not only affect climate, but also health and food security.



Source: Tai et al., 2014

Introduction

The increasing trend of Ozone (O_3)



Source: IPCC AR6, 2021

Particularly, Brewer-Dobson circulation over the tropics.

Several points to study:

- Stra-trop O_3 interaction
- VOC from oil/gas industry
- Long-range transport
- Reaction with PAN*
- Role of climate change
- Wildfire

Ref.: TOAR, 2019

*Peroxyacetyl nitrate (PAN): reservoir of NO_x that contributes to rural O_3 bloom.

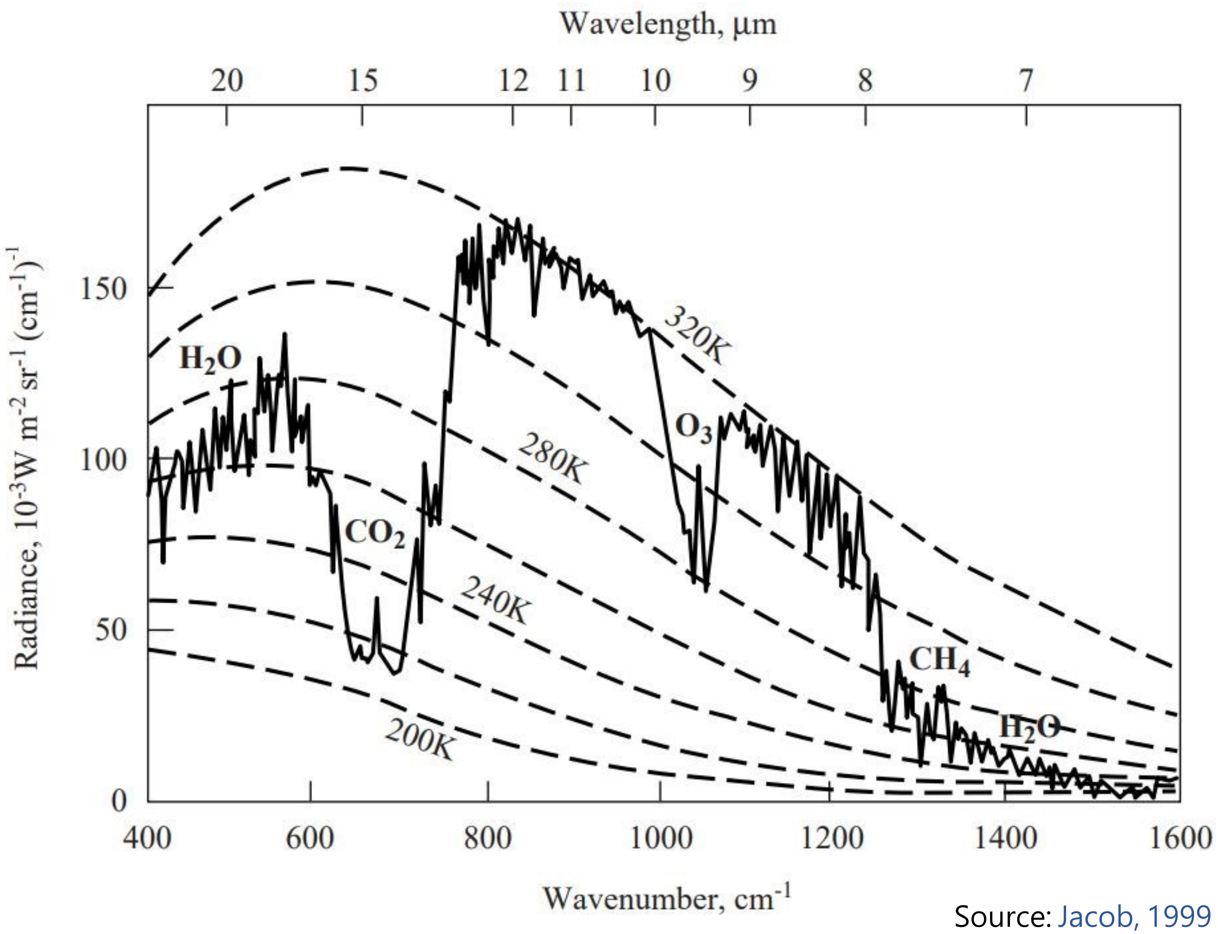
For this purpose, global-scale obs. is required

∴ Satellite observation

Background

Satellite observations: how and what

- O_3 absorption spectrum
  - Thermal infrared (TIR) ~ 9.5 µm
  - GOSATs: L1 product (raw data)
- Retrieval: Inverse method
  - Optimal estimation (commonly used)
  - Key reading: Rodgers (2000)
- Radiative transfer model (RTM)
  - Works as forward model (E.g., GFIT)
  - GFIT retrieves trace gases, GFIT2 applies optimal estimation, GFIT3 includes scattering effects of aerosol



Source: Jacob, 1999

A sample radiance spectrum over Africa in early 1970s

Some theoretical basics of retrieval (to my understanding)

Based on Inverse method by Rodgers (2000) and explanation in Brasseur & Jacob (2017)

- Finding the optimal estimation of state vector **x** by observation **y** and forward model **F(x)**

$$\boldsymbol{y} = \boldsymbol{F}(\boldsymbol{x}) + \boldsymbol{\varepsilon_0}$$

- By Bayes theorem, find the maximum of P(**x**|**y**) or the minimum of the cost function J(**x**)

$$P(\boldsymbol{x}|\boldsymbol{y}) = \frac{P(\boldsymbol{y}|\boldsymbol{x})P(\boldsymbol{x})}{P(\boldsymbol{y})}$$

The pdf in scalar form:

$$P(\boldsymbol{x}|\boldsymbol{y}) = \exp\left[-\frac{(x - x_A)^2}{2\sigma_A^2} - \frac{(y - kx)^2}{2\sigma_O^2}\right]$$

In vector form:

$$-2\ln P(\boldsymbol{x}|\boldsymbol{y}) = (\boldsymbol{x} - \boldsymbol{x}_A)^T \boldsymbol{S}_A^{-1}(\boldsymbol{x} - \boldsymbol{x}_A) + \left(\boldsymbol{y} - \boldsymbol{F}(\boldsymbol{x})\right)^T \boldsymbol{S}_O^{-1}\left(\boldsymbol{y} - \boldsymbol{F}(\boldsymbol{x})\right) + \boldsymbol{c}_3$$

- By finding the $\boldsymbol{\nabla}_{\boldsymbol{x}} J(\boldsymbol{x}) = 0$, we get:

$$\hat{\boldsymbol{x}} = \boldsymbol{A}\boldsymbol{x} + (\boldsymbol{I}_n - \boldsymbol{A})\boldsymbol{x}_A + \boldsymbol{G}\boldsymbol{\varepsilon}_O$$

I_n is identical matrix, **A** is the averaging kernel matrix, **G** is the gain matrix, **x** is "true" state

- x_A is <u>the prior estimate</u>: climatological mean, reanalysis data

- These information are important for **assessment** and **error analysis** of the retrieval

Notes: P(x|y) is the probability of x when y is true. **Bolded variables** are vectors.

Rodgers, C. D. (2000). *Inverse methods for atmospheric sounding: Theory and practice*. Singapore: World Scientific.
Brasseur, G. P. & Jacob, D. J. (2017). *Modeling of atmospheric chemistry Chapter 11*. Cambridge, UK: Cambridge University Press.

Some theoretical basics of retrieval (to my understanding)

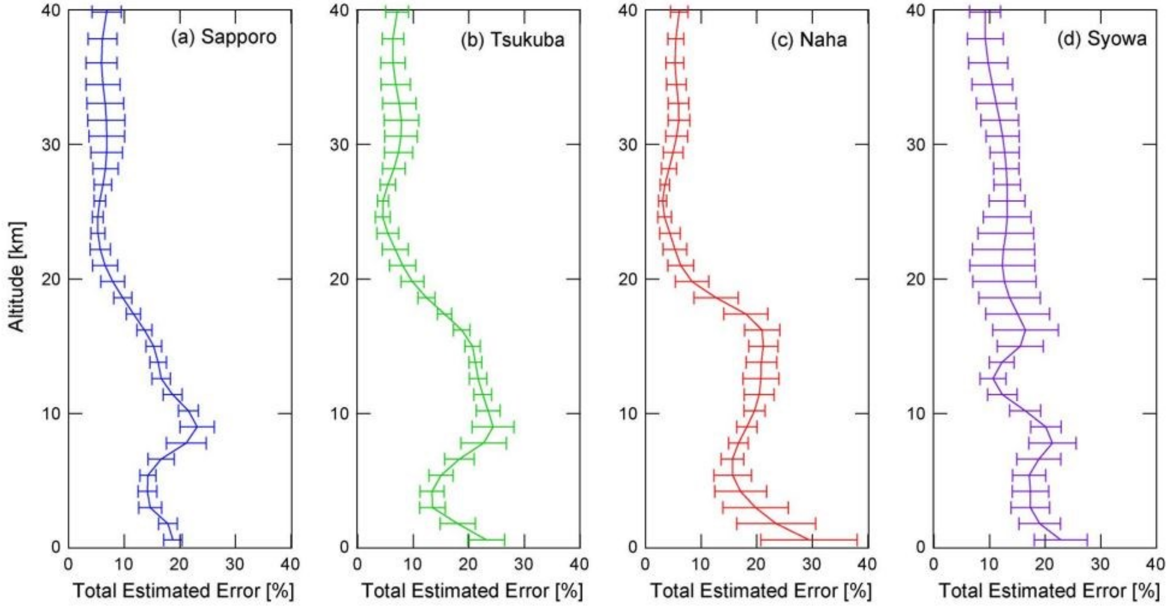
- Error analysis for retrieval
  - Difference between retrieval (state vector) **x** and the true state vector **x** (sondes or models)
  - The error covariance matrix:

$$\hat{\boldsymbol{S}} = (\boldsymbol{I_n} - \boldsymbol{A})\boldsymbol{S_A}(\boldsymbol{I_n} - \boldsymbol{A})^T + \boldsymbol{G}\boldsymbol{S_O}\boldsymbol{G}^T$$

  - The largest should be **smoothing error** comes from limited vertical resolution
  - The **observational error**
    - the sum of S_I, S_R, S_M

An example from Ohyama et al. (2012), the estimated errors of GOSAT retrieval is shown:

- Mainly smoothing error
- Secondly measurement (obs.) error
- And others



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Review of infrared sounders

Brief introduction of physical background

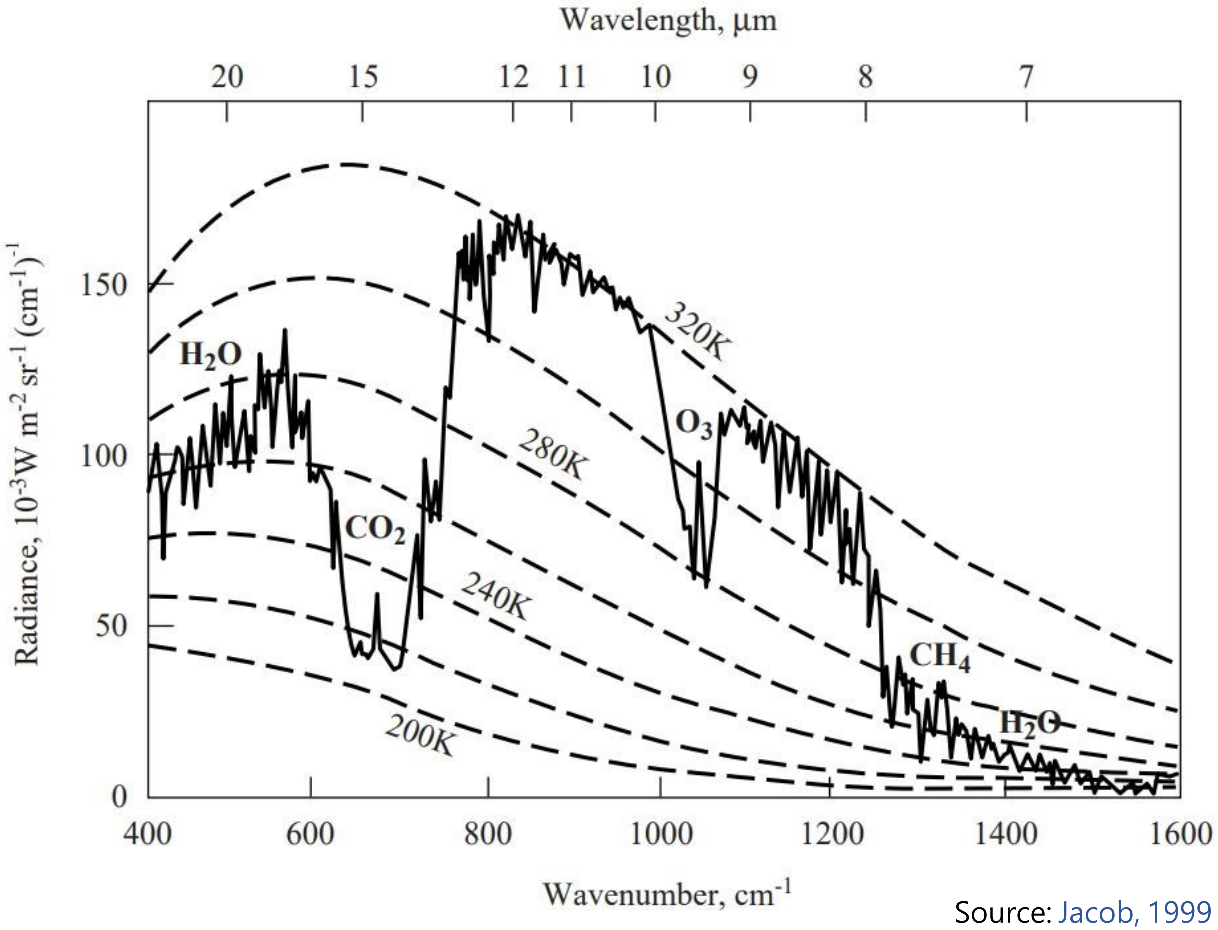
- O_3 absorption spectrum
  - Thermal infrared (TIR) ~ 9.5 µm

- Sun-syn. and passive sensor

Validation methods

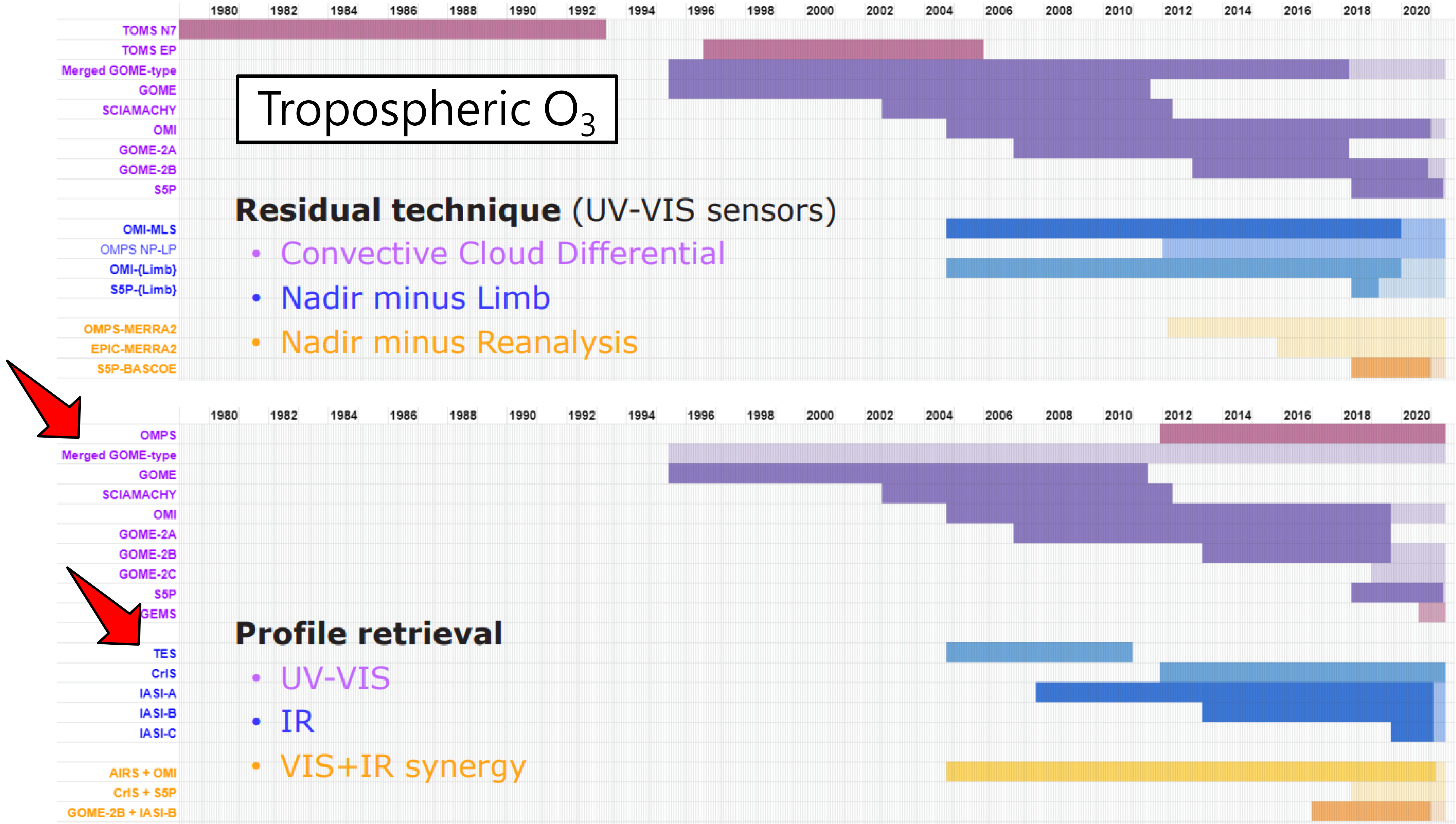
- Ozonesonde
- Validated sensor
- Ground-based obs.
- Chemical transport model (CTM)

Source: NOAA, 2020



Source: Jacob, 1999

A sample radiance spectrum over Africa in early 1970s



Source: Hubert et al., 2022 on AC-VC-18 meeting (online)

Intercomparison of sensors and models

Ideas for meaningful validation

- Validation and Intercomparison of satellites and CTMs (Zhang et al., 2010)
  - In-situ method: ozonesonde validation (limitation: spareness of sites)
  - CTM method: use CTM field by field comparison
  - Averaging kernel smoothing method: smooth "B" use "A" AK, can be sensors

e.g., use IASI to validate TROPOMI

- Either case: avoid direct comparison
  - Pre-processing: AK smoothed sonde & synthetic atmosphere (CTM)

- Key references
  - Rodgers & Connor (2003): intercomparison of sensors
  - Zhang et al. (2010): intercomparison of sensors and CTMs

Intercomparison of sensors and models

Metrics for assessing the performance of sensor and model

- Degree of freedom of signal (DOFS): the reduction of variance by obs.

$$DOFS = n - \sum_{i=0}^{n} \frac{\hat{\sigma_i}^2}{\sigma_{A,i}^2} = \sum_{i=1}^{n} \frac{\sigma_{A,i}^2 - \hat{\sigma_i}^2}{\sigma_{A,i}^2}$$

It is quantifying how well our observations have reduced uncertainty of the prior estimate. **Smaller variance of retrieval, larger the reduction of uncertainty.**

- Root-mean square error (RMSE): like the SD of mea. referring to obs.

$$RMSE = \left[\frac{1}{N}\sum_{i=1}^{N}(M_i - O_i)^2\right]^{\frac{1}{2}}$$

Recall the definition of SD:

$$\sigma_M = \left[\frac{1}{N}\sum_{i=1}^{N}(M_i - \bar{M})^2\right]^{\frac{1}{2}}$$

- Mean bias (BIAS): difference between mea. (or retrieval) and obs.

$$BIAS = \frac{1}{N}\sum_{i=1}^{N}(M_i - O_i) = \bar{M} - \bar{O}$$

Rodgers, C. D. (2000). *Inverse methods for atmospheric sounding: Theory and practice*. Singapore: World Scientific.
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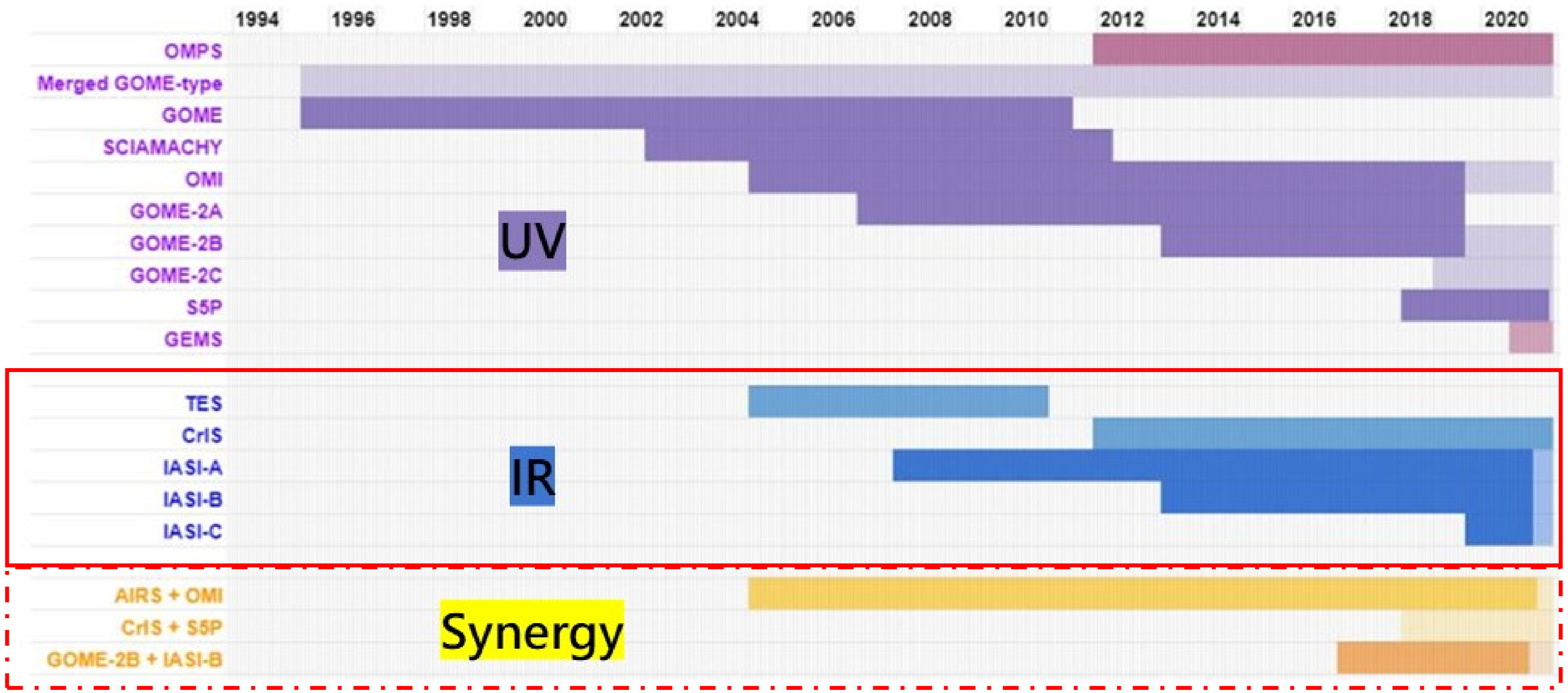
Review of infrared sounders

Summary of scientific findings and methodology

- In chronological order: TES, IASI, CrIS, synergy of sensors (some)
  - This presentation: UV sensors will be neglected, except TROPOMI

- Indeed, Atmospheric Infrared Sounder (AIRS) is the earliest IR sounder (since 2002), but only total column is published.



Synergy of AIRS + OMI

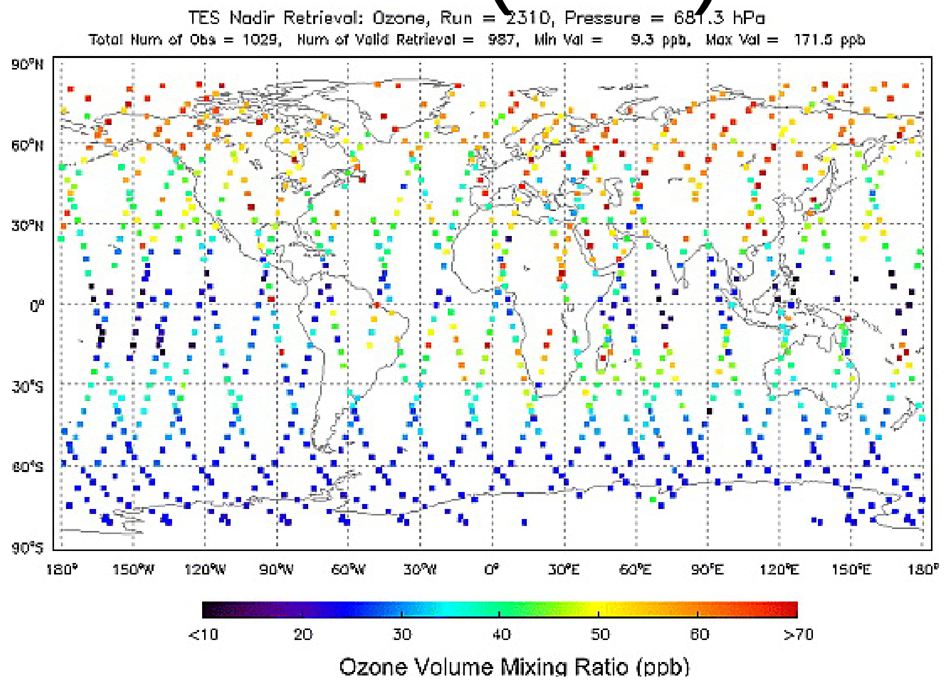
Tropospheric Emission Spectrometer (TES)

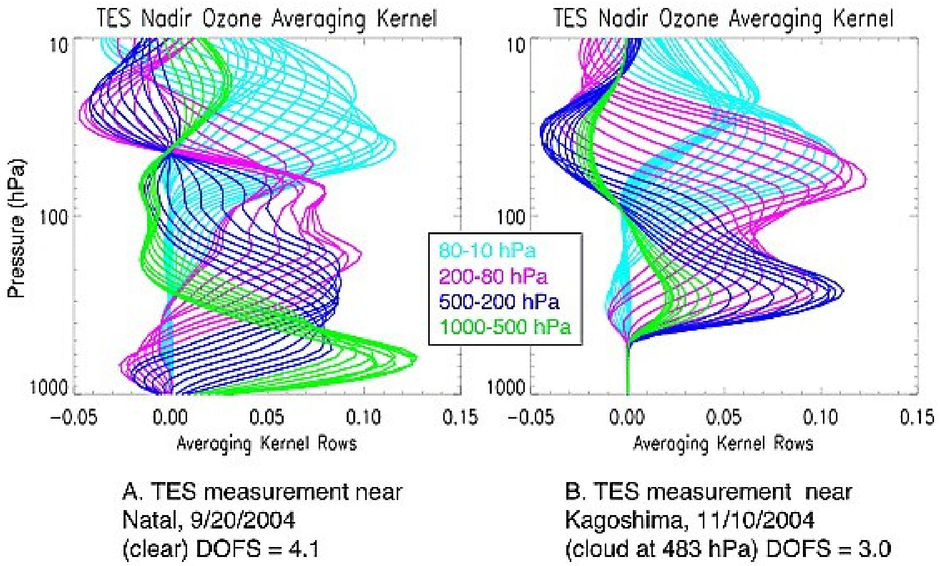
- Onboard NASA Aura since 2003
  - With MLS, OMI and other
  - 16-day repeating cycle, sun-synchronous
  - Retired in 2018
- Validation has been made by comparing to:
  - Ozonesonde (Worden et al., 2007; Nassar et al., 2008)
  - NASA DC-3 aircraft (Richards et al., 2008)
  - GEOS-Chem CTM (Luo et al., 2002)
- Polar surface O_3 retrieval (Boxe et al., 2010)
  - Artic Intensive Ozonesonde Network Study (ARICONS)

[Upper, Lower trop.]	Mid-latitudes (25° > λ > 60°)	Tropics (λ < 25°)
Bias	[16.79, -2.57]	[9.80, -7.35]
Root-mean-square difference (RMS)	[18.93, 6.66]	[10.26, 7.01]

※ 19 sonde sites are used.

Source: Worden et al., 2007

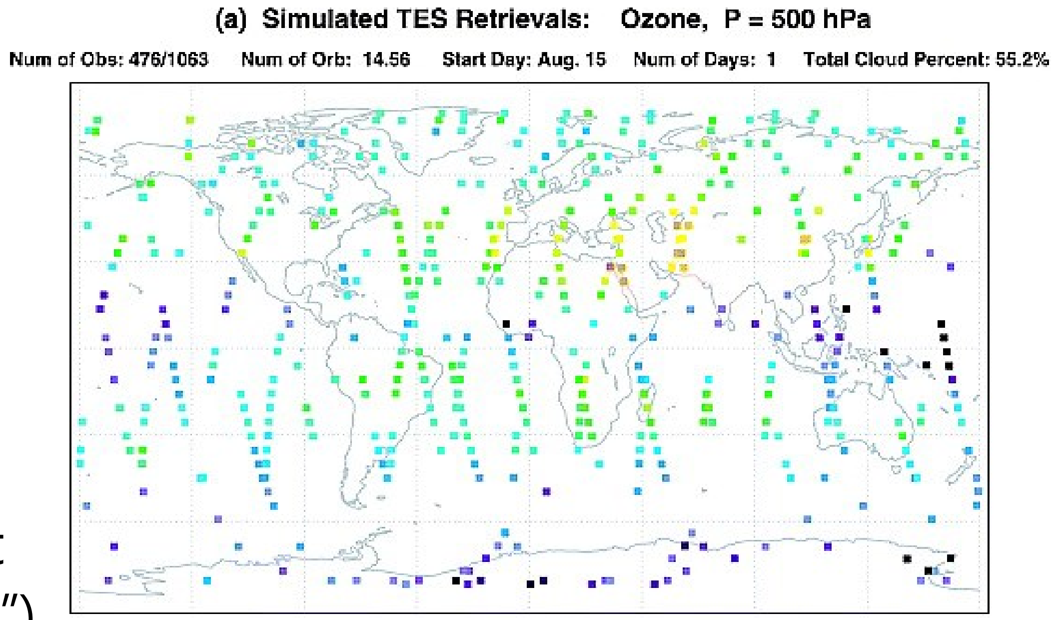


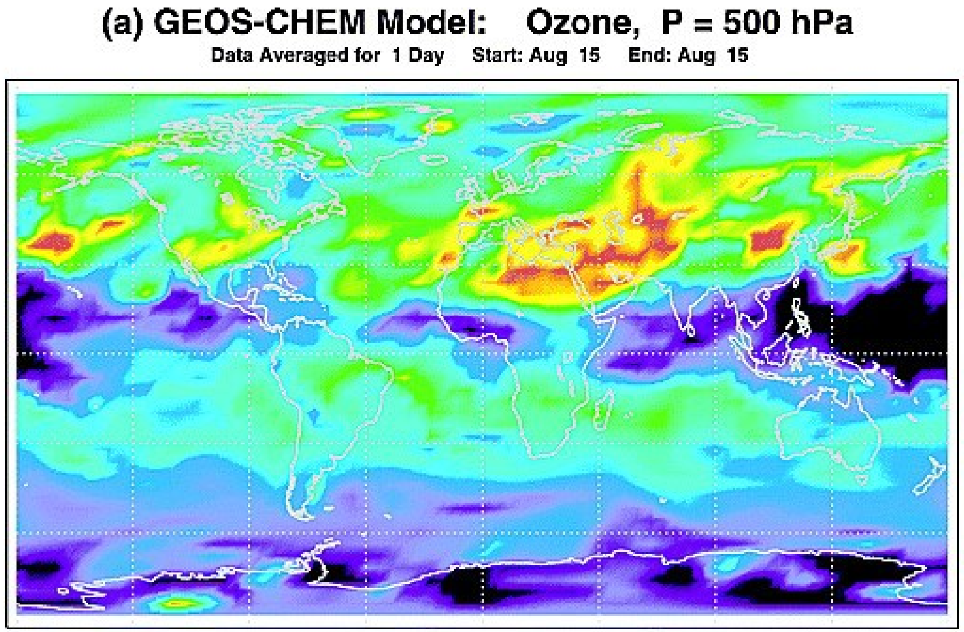


Source: Worden et al., 2007

Tropospheric Emission Spectrometer (TES)

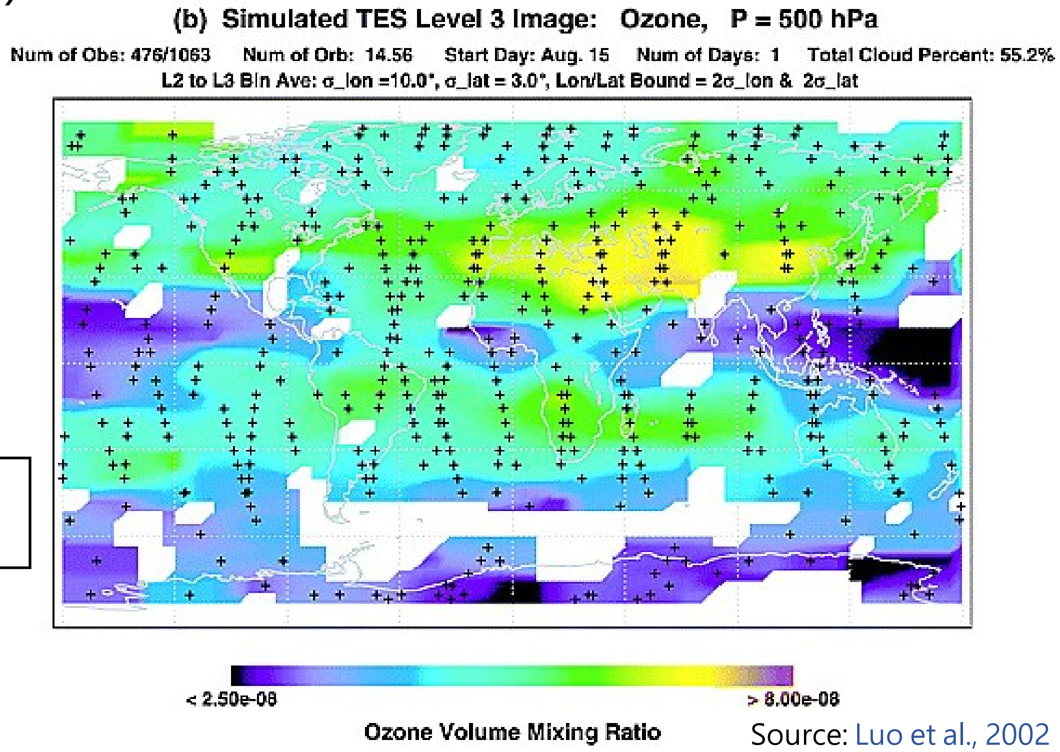
- A validation by GEOS-Chem (Luo et al., 2002)
  - Use GEO-Chem as a synthetic atmosphere
- Procedure of validation
  - Model “cloudy condition” is rejected along footprint
  - Retrieval referring to synthetic atmosphere (“Level 2”)
  - Interpolate global map (“Level 3 products”)





75% area: <10% error
15% area: 10-20% error

※ Comparing to model output.



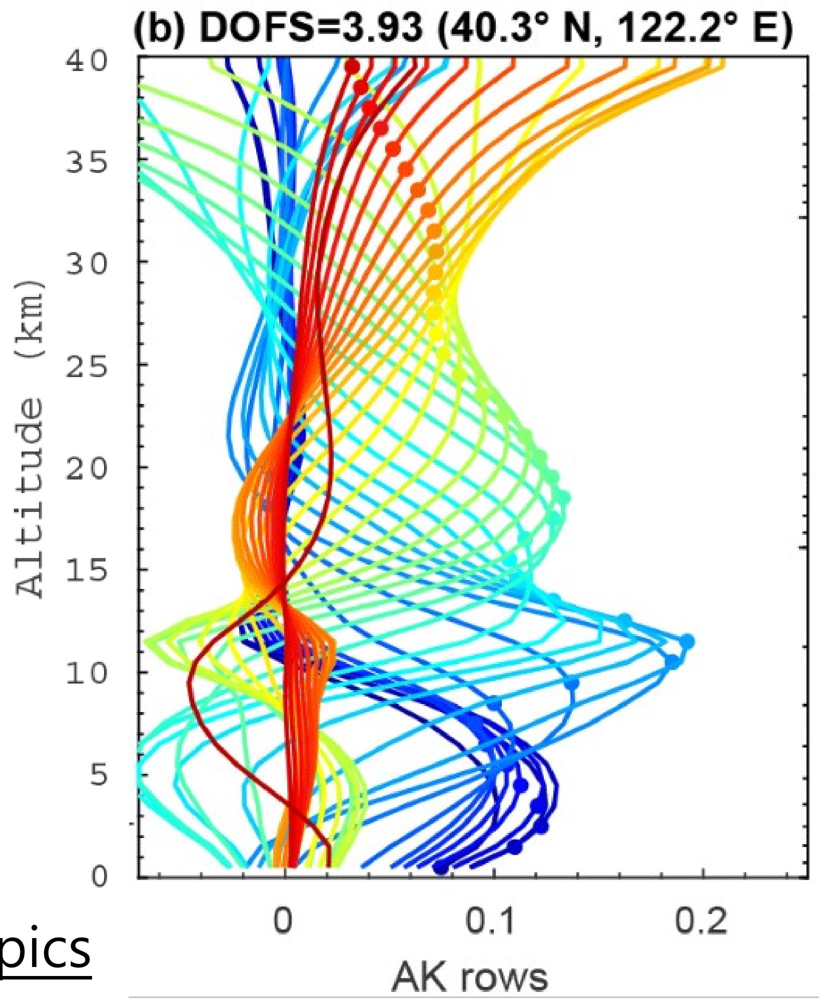
Source: Luo et al., 2002

Infrared Atmospheric Sounding Interferometer (IASI)

- Onboard EAS MetOp series since 2006
  - With GOME-2 (UV sensor)
  - 29-day repeating cycle, sun-synchronous

- Validation by Boynard et al. (2016, 2018):
  - 5%-19% bias (see below)
  - Excellent agreement with GOME-2
  - IASI-A and IASI-B: <2.4%, after 2015 <1.4%
  - Dufour et al. (2012): 10%-20% for lower-troposphere

- By comparing to AK smoothed sonde:
  - Maximum bias in "upper-trop.-lower-strat." (20%-40%)
  - Underestimate 11%-13% in midlatitudes, 16%-19% in tropics
  - Overestimate 4%-5% in high latitudes



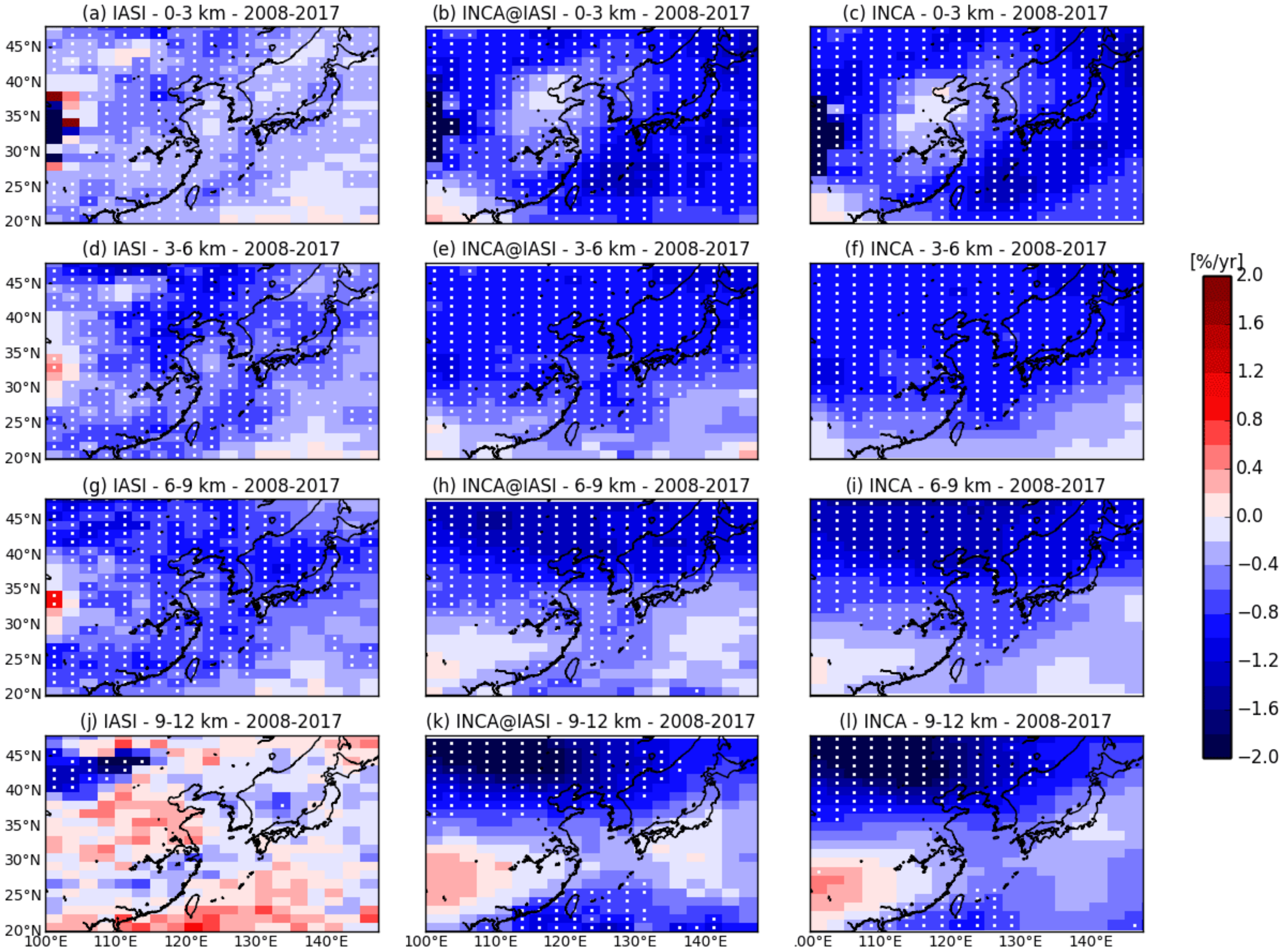
Source: Boynard et al., 2018

Infrared Atmospheric Sounding Interferometer (IASI)

- Some application:
  - Ozone peak by anticyclone in Mediterranean basin (Doche et al., 2014)
  - Urban source of Ozone (Dufour et al., 2010, 2021)
  - VOC by neural network retrieval framework (Franco et al., 2018, 2019, 2020)

- Urban source of Ozone (Dufour et al., 2021)
  - IASI retrieval & INCA model
  - Smoothing INCA by AK (?)

- Validation method
  - AK smoothing of sonde and aircraft data



※ White dots are statistically significant at 5%

Source: Dufour et al., 2021

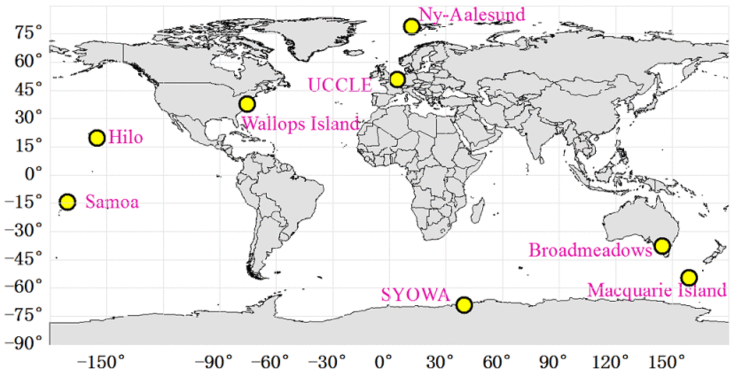
Cross-track Infrared Sounder (CrIS)

- Aboard Suomi-NPP NOAA since 2011
  - With OMPS and other
  - 16-day repeating cycle, sun-syn.

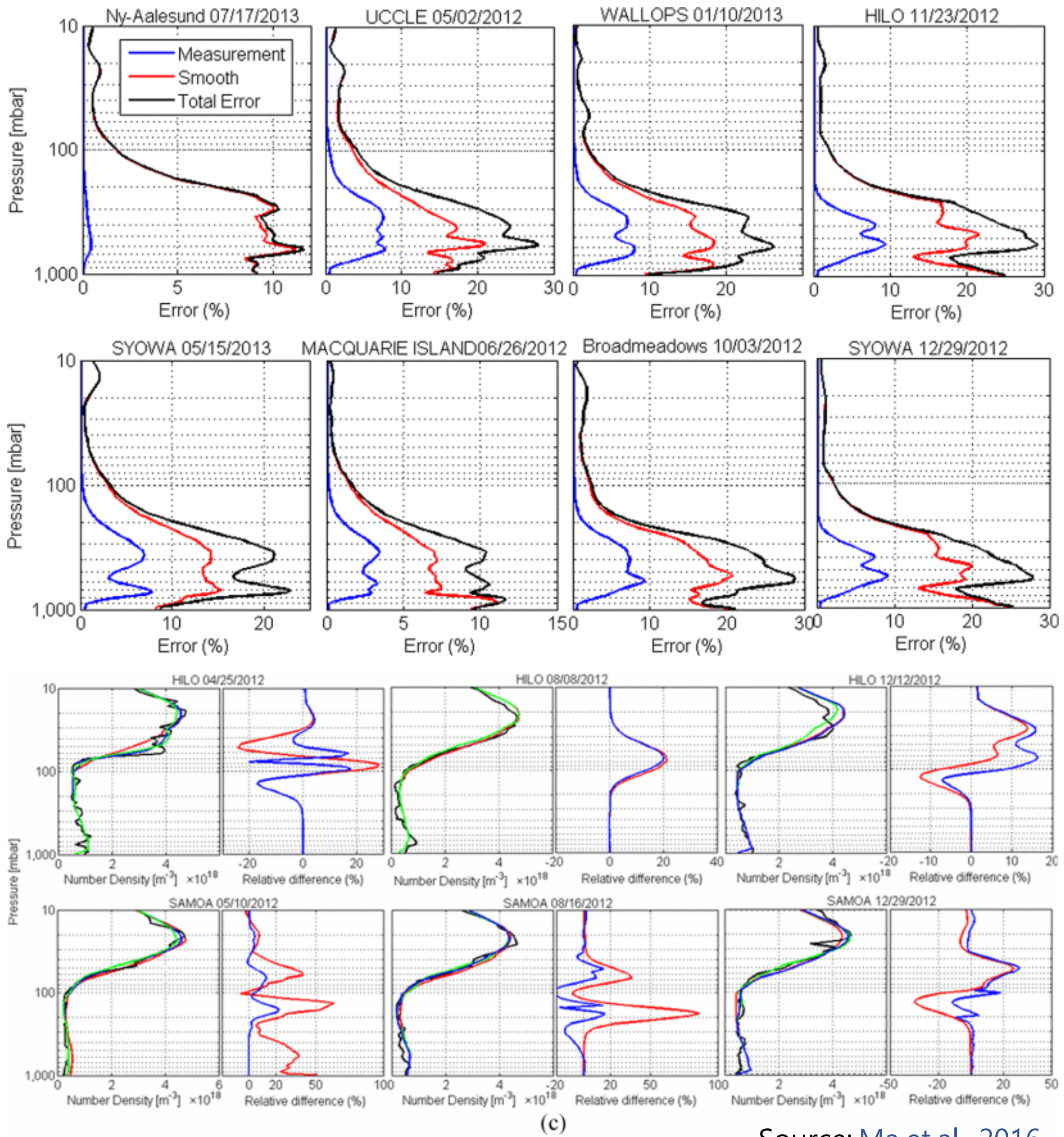
- Validation by Ma et al. (2016)
  - 8 ozonesonde sites with AK smoothed data
  - Errors are high in mid-troposphere

Smoothing error
- Predominates
- Lower Trop.

- Applications
  - First isoprene (BVOC) retrieval by Fu et al. (2019)
  - VOC retrieval and machine learning (Franco et al., 2018, 2019, 2020; Wells et al., 2020, 2022)
  - PAN formation (Calahorrano et al., 2021)
  - Synergy with TROPOMI for ozone retrieval



Tropical regions:
- STE causes uncertainty



Source: Ma et al., 2016

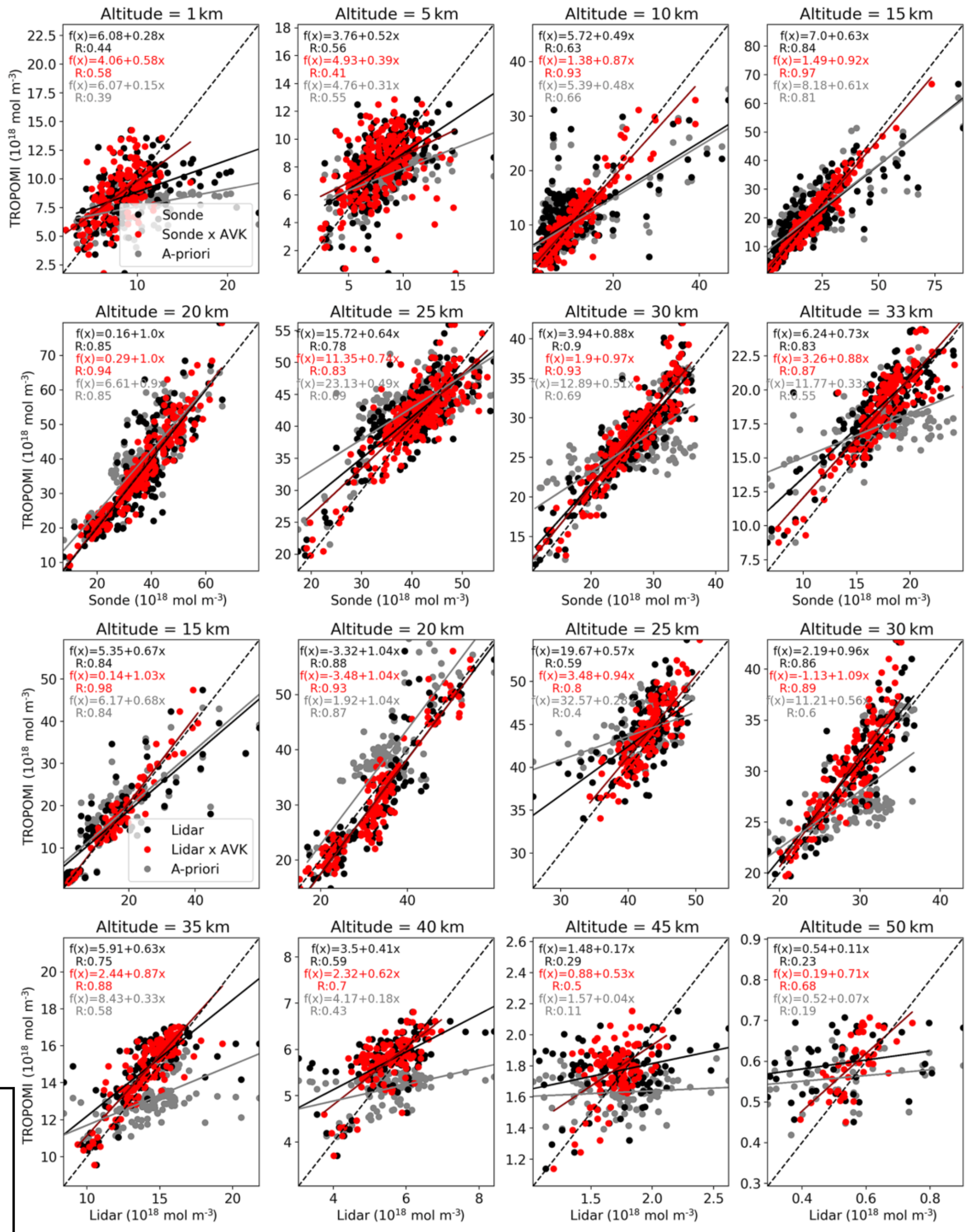
TROPOspheric Monitoring Instrument (TROPOMI)

- Aboard Sentinel-5 Precursor since 2017
  - High-resolution: 3 km x 5.5 km
  - Ozone retrieval in UV band
  - 16-day repeating cycle, sun-syn.

- Applications
  - Ozone retrieval in UV band (Mettig et al., 2021)
  - Synergy with CrIS (Mettig et al., 2022)

- Validation (Mettig et al., 2021)
  - Sonde and lidar (Pearson's r)
  - Bias and RMSE are unknown

Red: with AK smoothing
Black: without AK smoothing
Grey: A Priori vs sonde

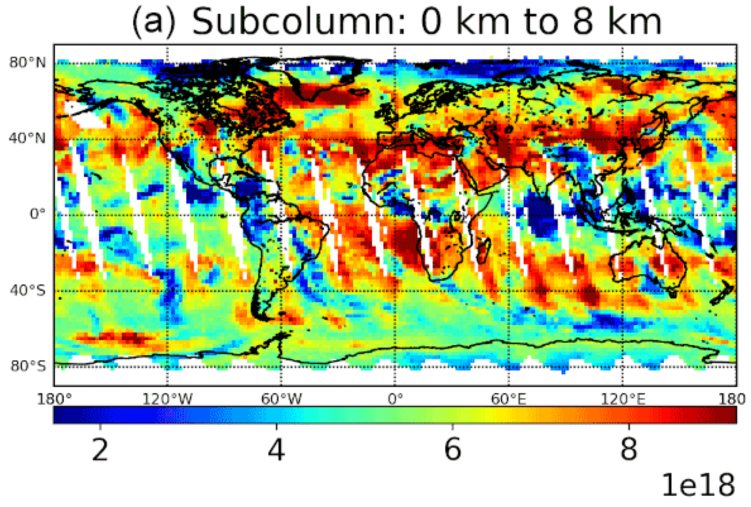


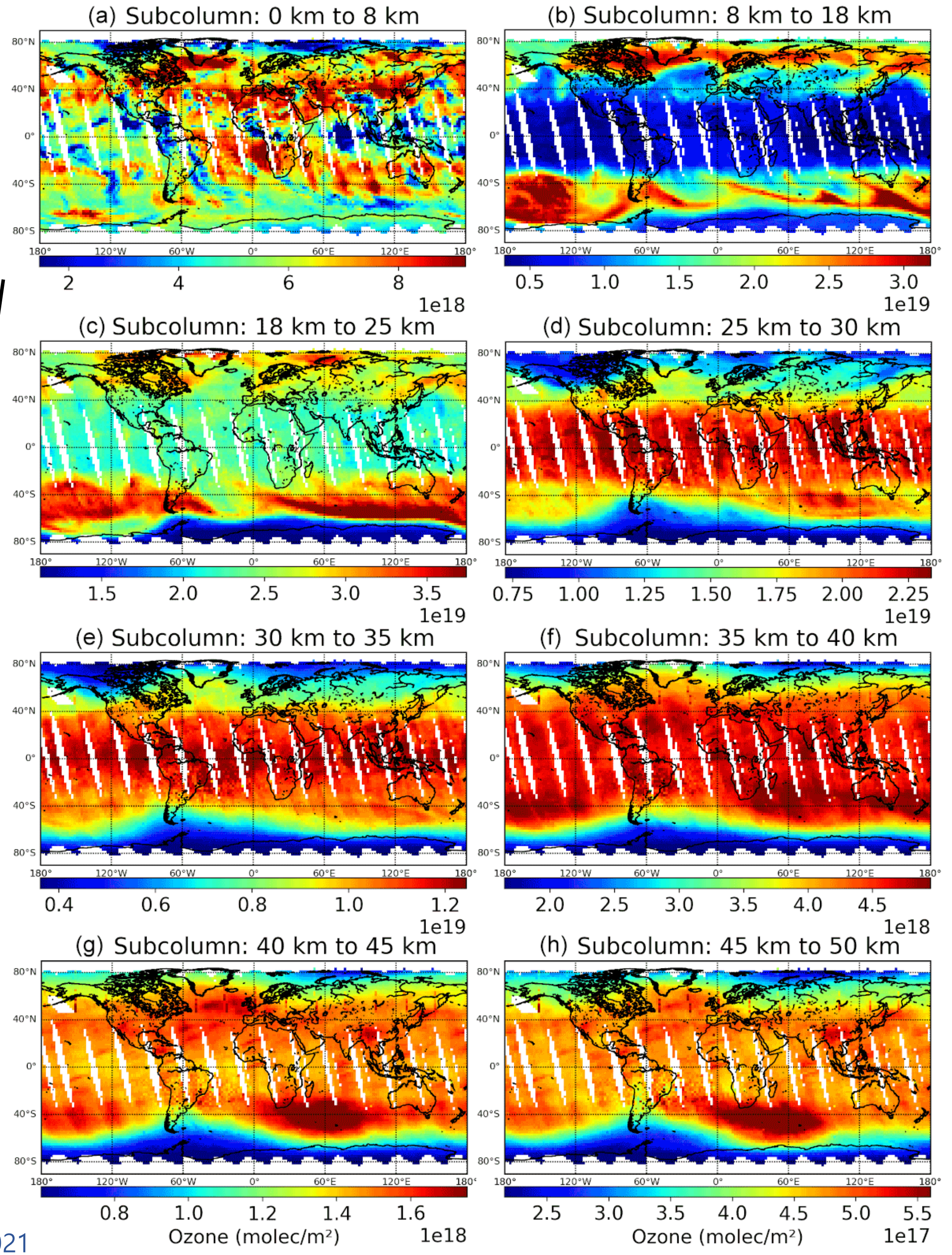
Source: Mettig et al., 2021

TROPOspheric Monitoring Instrument (TROPOMI)

- Applications
  - Ozone retrieval in UV band (Mettig et al., 2021)
  - Synergy with CrIS (Mettig et al., 2022)

- Validation (Mettig et al., 2021)
  - Sonde and lidar (Pearson's r)
  - UTLS Bias: -5% to +5% for all latitudes (UTLS)
  - LT Bias: ~10% (~20% in tropics and high lat.)

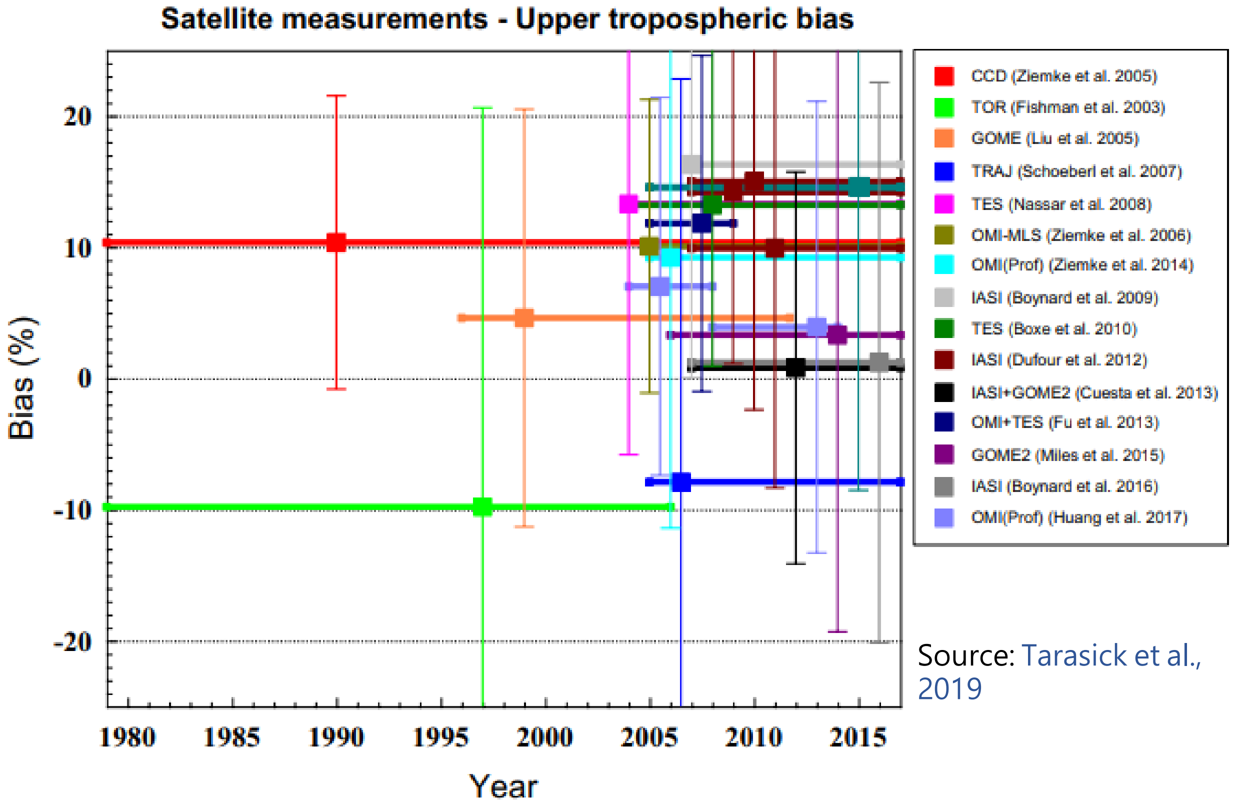




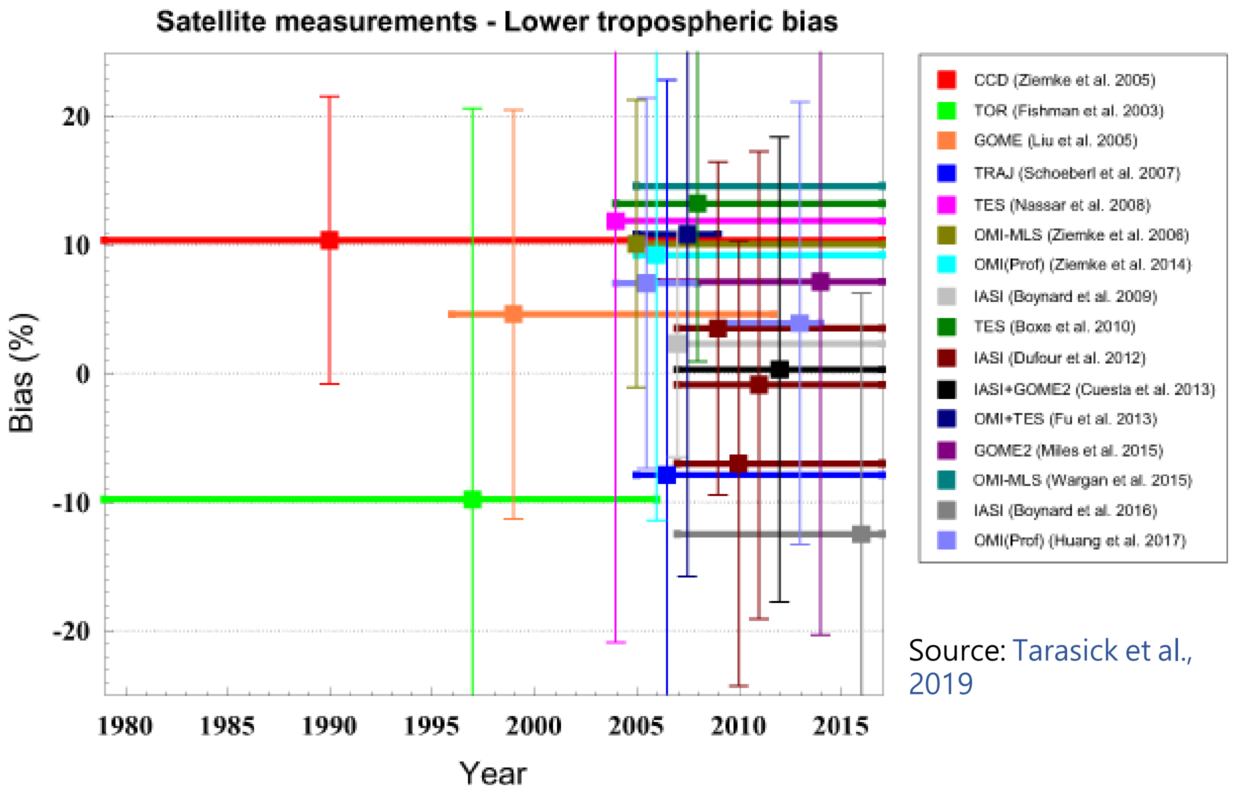
Source: Mettig et al., 2021

Synergy of sensors: IASI + GOME-2

- Range of bias: -10% to +15%
  - IASI + GOME2: 1% (Cuesta et al., 2013)
- Among IR sounders, IASI has the lowest bias



Source: Tarasick et al., 2019



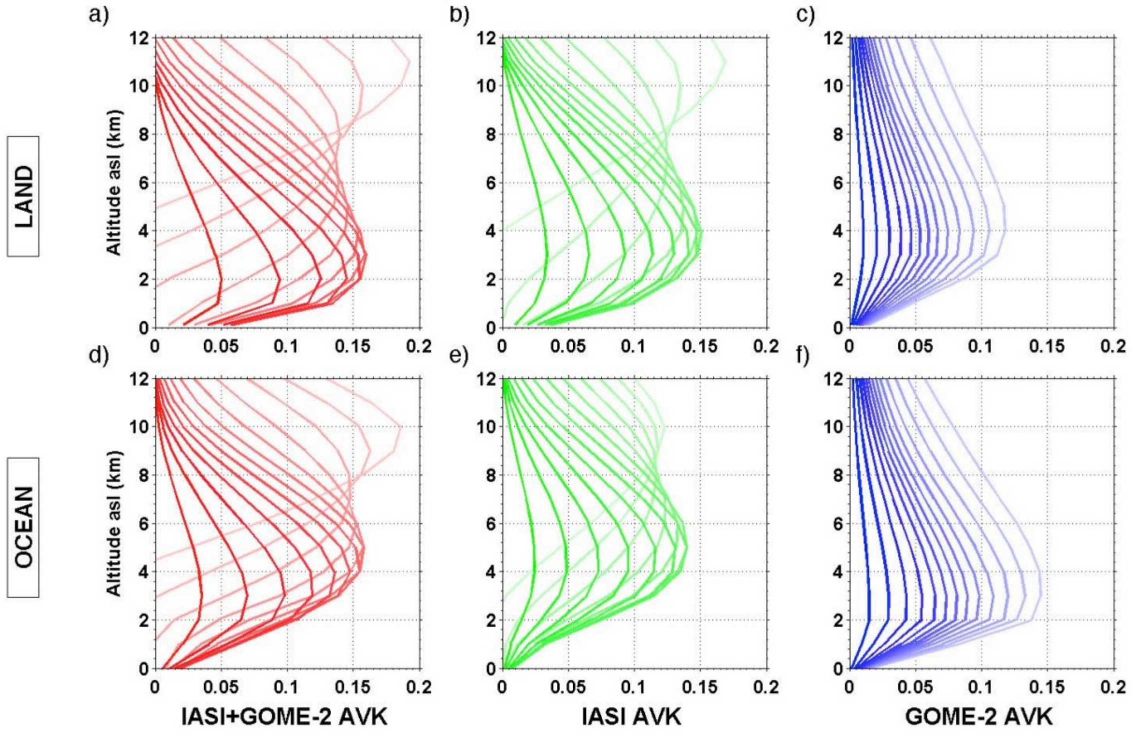
Source: Tarasick et al., 2019

Synergy of sensors: IASI + GOME-2

- There are plenty of combinations (e.g., CrIS+TROPOMI, TES+OMI, AIRS+OMI etc)
  - Mostly combination of TIR + UV sensors
  - Mostly nadir sensors, but some nadir + limb view (e.g., SUNLIT)
  - Mostly from same satellite platform (e.g., AIRS + OMI from AURA)

- IASI + GOME-2 (Cuesta et al., 2013)
  - 50% improvement of DOFS
  - UV and TIR spectrum are combined
  - Better correlation and lower RMSE

Unsolved issue: very low (<0.02) AK sensitivity near the surface.



Source: Cuesta et al., 2013

Synergy: IASI + GOME-2

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  - 50% improvement of DOFS
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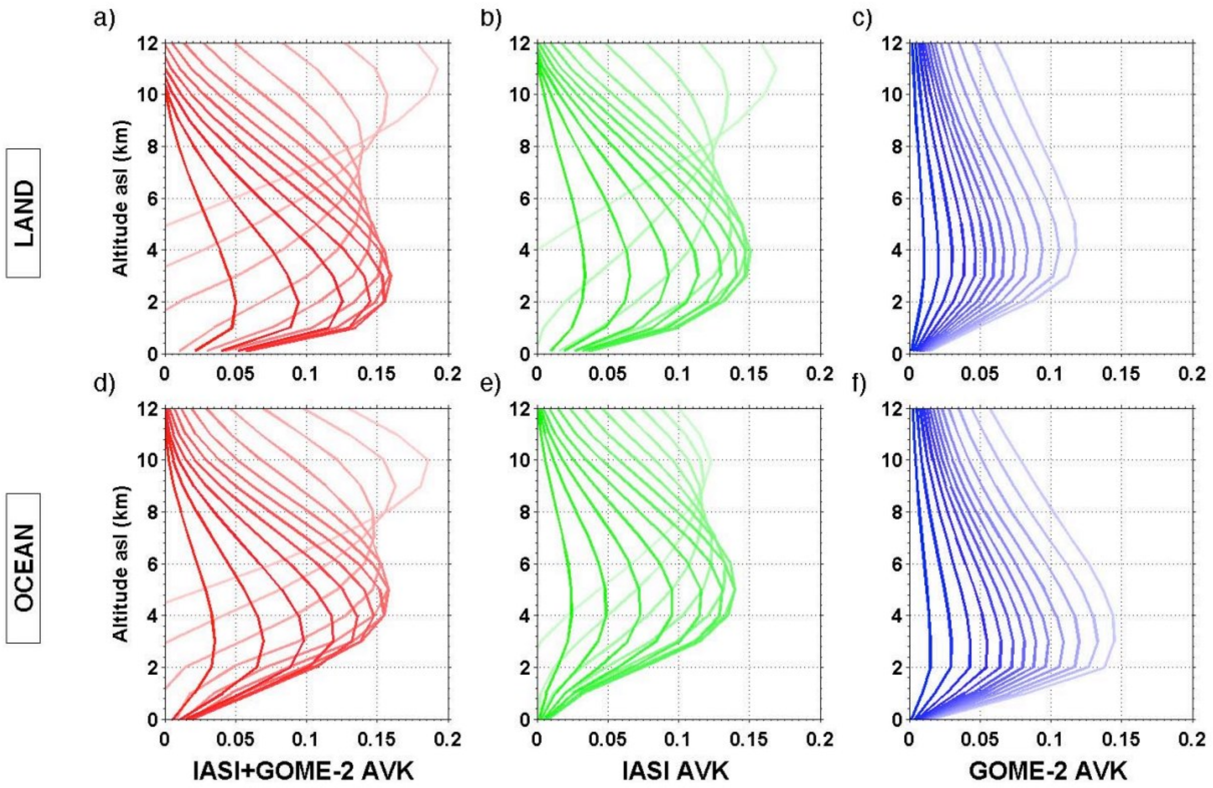
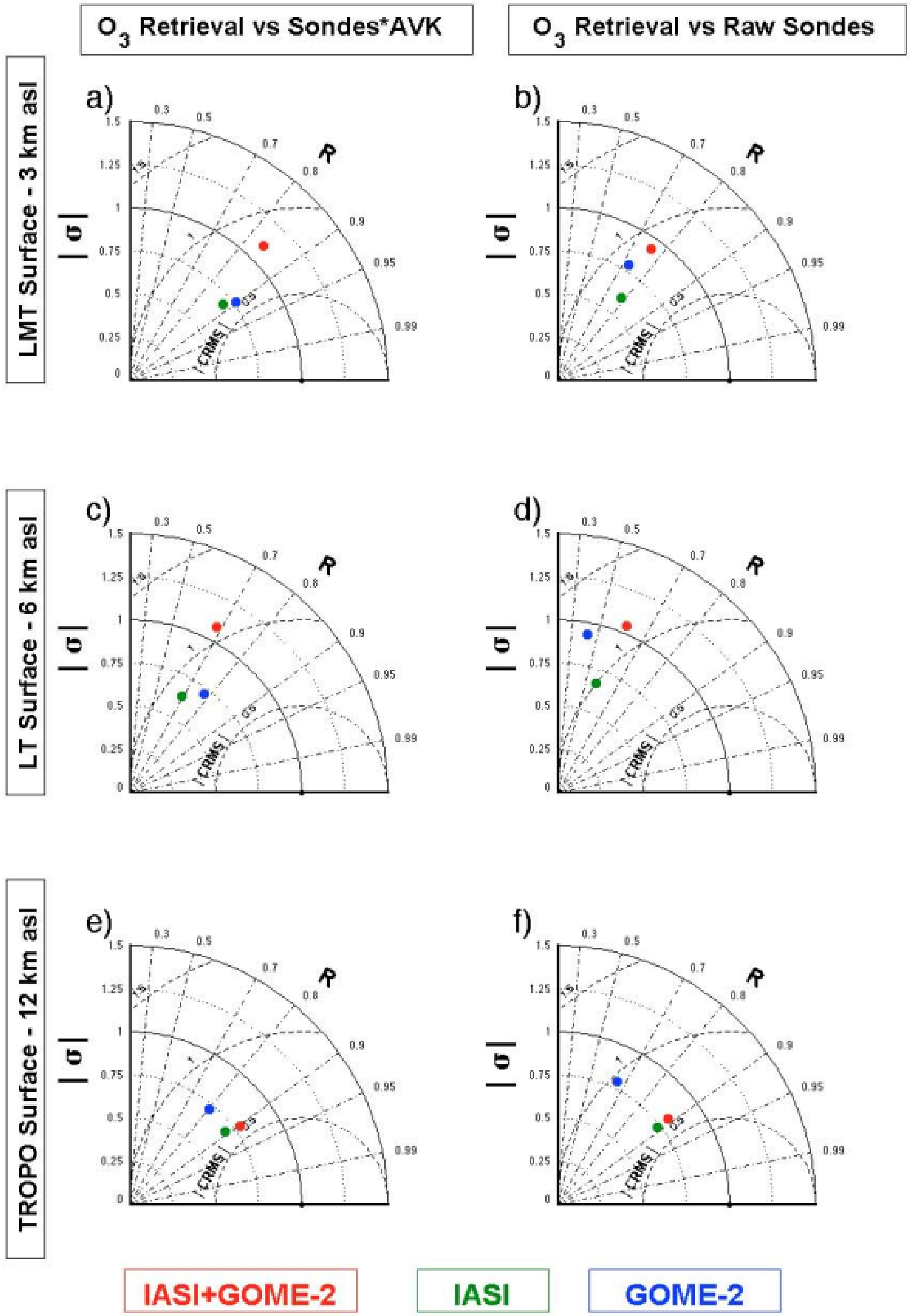


Source: Cuesta et al., 2013

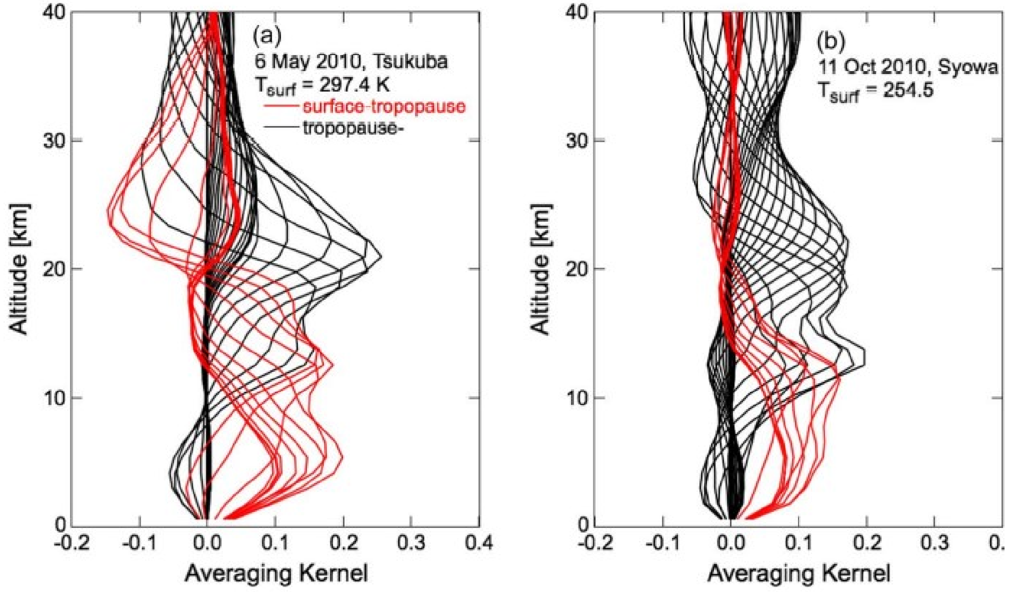


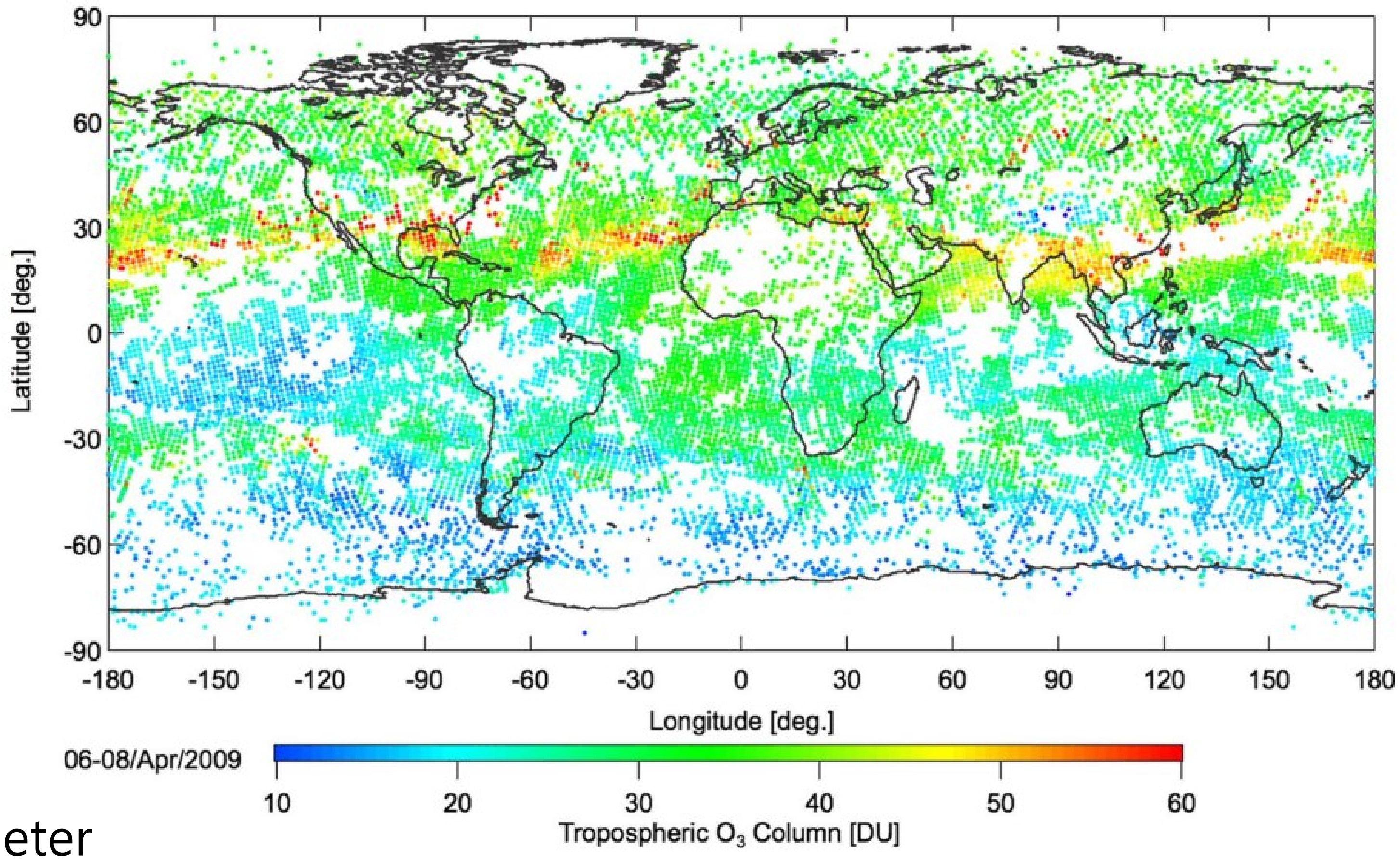
Source: Cuesta et al., 2013

Extra: TROPESS

- TRopospheric Ozone and its Precusors from Earth System Sounding (TROPESS) project
  - Aim to build a continuous record of Ozone and other constituents
  - Initiated by NASA
- Earth System Data Records (ESDRs)
  - Multiple sources (sensors) using common retrieval algorithm
    - L1B products from AIRS, OMI, TROPOMI, CrIS, OMPS
  - Consists of O_3, PAN, CH_4 etc
  - Data format: NetCDF
- Maybe it can be the <u>fourth validation method</u>

GOSAT

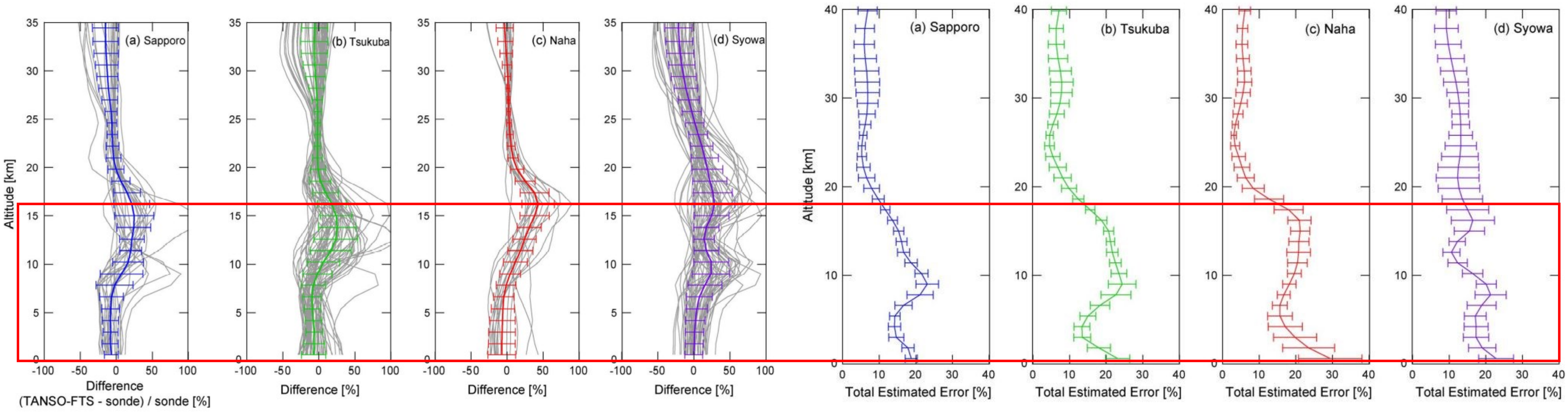




- By Ohyama et al. (2012)
- Validation: 4 sites in Japan
  - Ozonesonde and Dobson spectrometer
  - Error: 5%-10% depending on meteorological condition
  - DOFS: 3-4 (total column) and 0.5-2 (tropospheric)
  - Bias: 8.8 DU (3%)
  - RMSE: 10.9 DU (4.1%)

Next step by the authors: compare with other retrieval (no paper was found)

GOSAT



- Significant estimated error: 10%-30% at lower troposphere
- Low difference with AK smoothed sonde profile

- Error from (majorly) smoothing error
- It indicates that smoothed sonde could not explain true state well

Summary

- Intercomparison of sensors and models

- O_3 tropospheric chemistry
  - Global: Budget from CO, CH_4, Isoprene, NO_2, etc
  - Urban: PAN and industrial activity

- What've I done in last months?
  - Familiarising myself with the field through reading <u>textbooks and literatures</u>

- What's next?
  - Analysing GOSAT and GOSAT-2 data, retrieval, <u>**validation**</u>
  - Intercomparison with CTM, and tropospheric chemistry of ozone

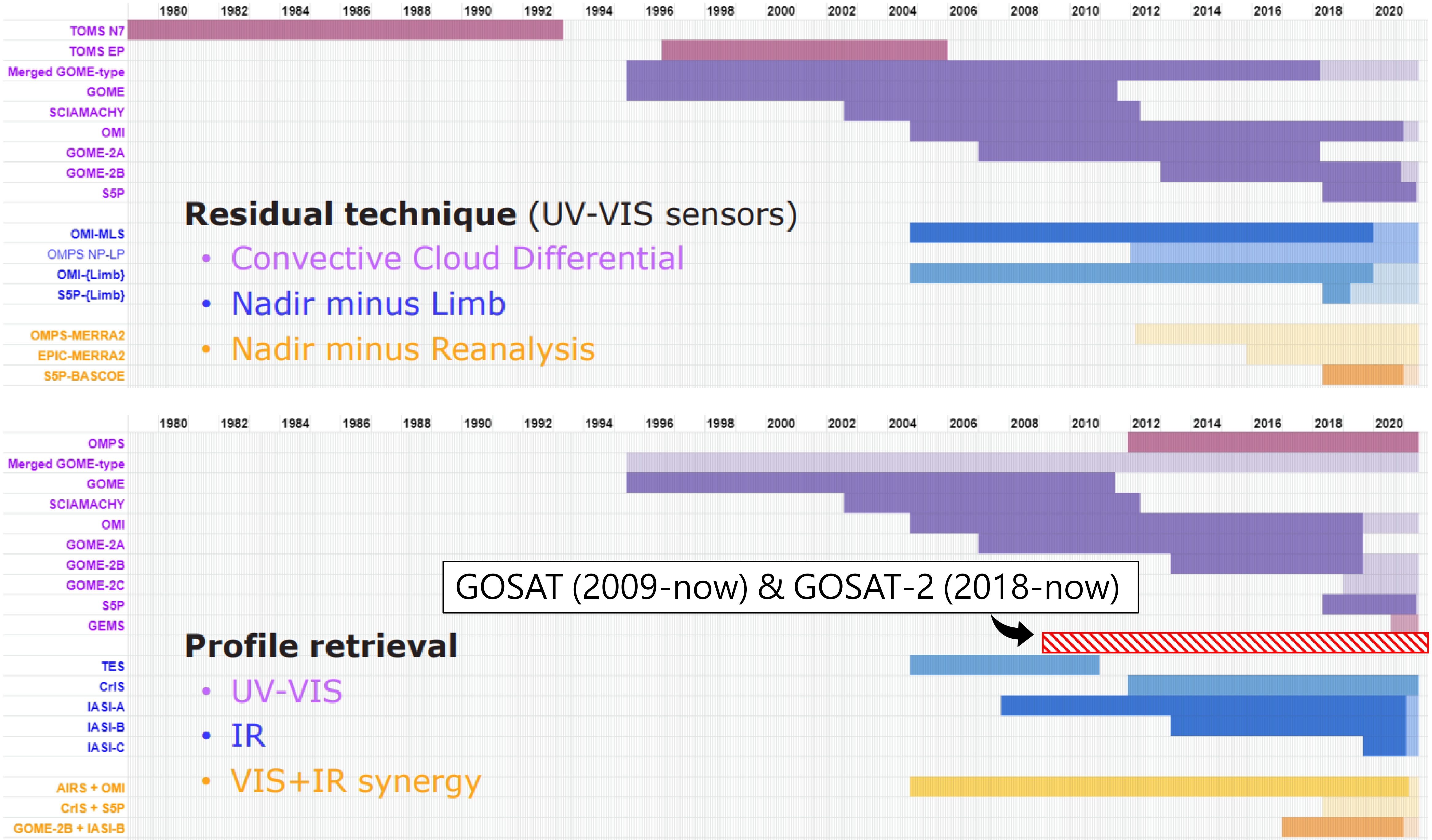
Several points to study:
- Stra-trop O_3 interaction
- VOC from oil/gas industry
- Long-range transport
- Reaction with PAN*
- Role of climate change
- Wildfire

Ref.: TOAR, 2019

*Peroxyacetyl nitrate (PAN): reservoir of NO_x that contributes to rural O_3 bloom.

WHY is tropospheric O3 increasing? (Reason)

HOW can we stop it? (Solution)



Source: Hubert et al., 2022 on AC-VC-18 meeting (online)

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- And others in next few pages

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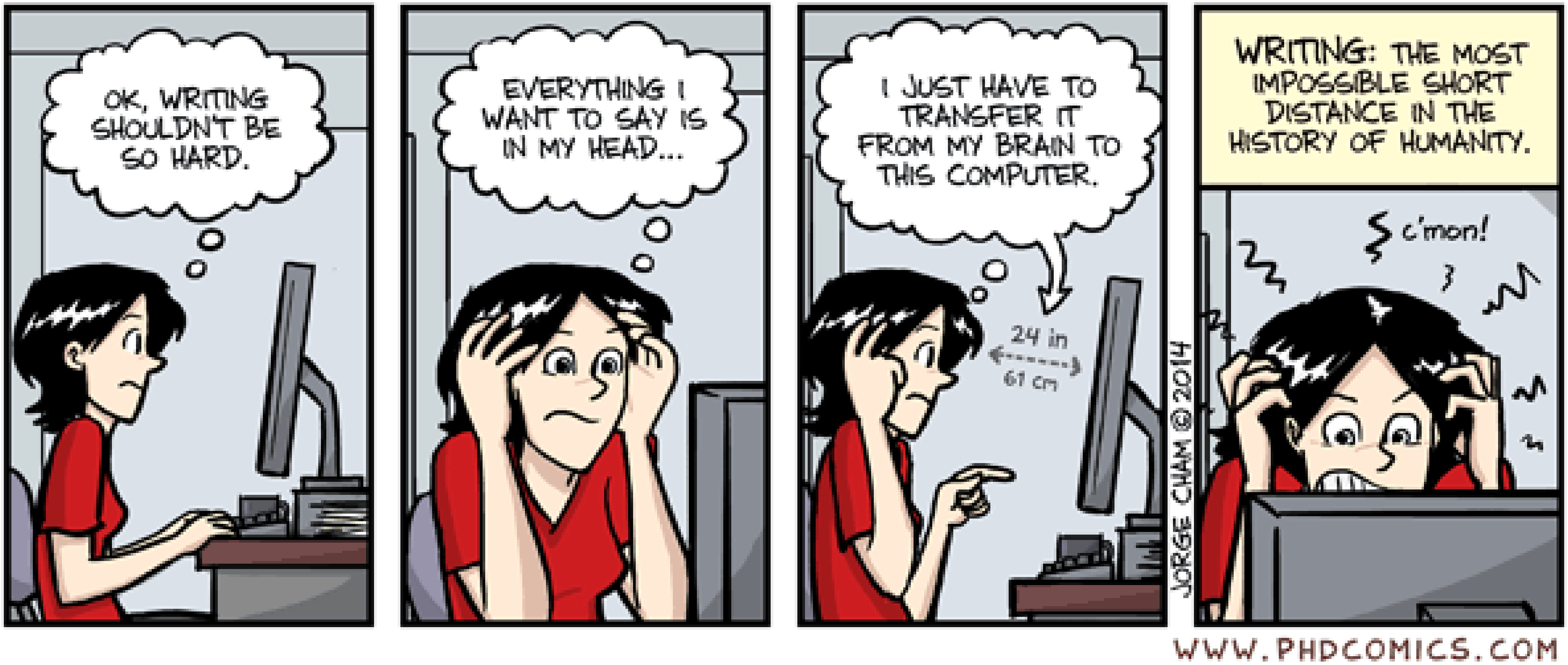

OK, WRITING SHOULDN'T BE SO HARD.
EVERYTHING I WANT TO SAY IS IN MY HEAD...
I JUST HAVE TO TRANSFER IT FROM MY BRAIN TO THIS COMPUTER.
24 in
61 cm
JORGE CHAM © 2014
WRITING: THE MOST IMPOSSIBLE SHORT DISTANCE IN THE HISTORY OF HUMANITY.
c'mon!
WWW.PHDCOMICS.COM

Terminology: data processing level by NASA

Data Level	Description
Level 0	Reconstructed, unprocessed instrument and payload data at full resolution, with any and all communications artifacts (e.g., synchronization frames, communications headers, duplicate data) removed. (In most cases, NASA's EOS Data and Operations System [EDOS] provides these data to the DAACs as production data sets for processing by the Science Data Processing Segment [SDPS] or by one of the SIPS to produce higher-level products.)
Level 1A	Level 1A (L1A) data are reconstructed, unprocessed instrument data at full resolution, time-referenced, and annotated with ancillary information, including radiometric and geometric calibration coefficients and georeferencing parameters (e.g., platform ephemeris) computed and appended but not applied to L0 data.
Level 1B	L1B data are L1A data that have been processed to sensor units (not all instruments have L1B source data).
Level 1C	L1C data are L1B data that include new variables to describe the spectra. These variables allow the user to identify which L1C channels have been copied directly from the L1B and which have been synthesized from L1B and why.
Level 2	Derived geophysical variables at the same resolution and location as L1 source data.
Level 2A	L2A data contains information derived from the geolocated sensor data, such as ground elevation, highest and lowest surface return elevations, energy quantile heights (“relative height” metrics), and other waveform-derived metrics describing the intercepted surface.
Level 2B	L2B data are L2A data that have been processed to sensor units (not all instruments will have a L2B equivalent).
Level 3	Variables mapped on uniform space-time grid scales, usually with some completeness and consistency.
Level 3A	L3A data are generally periodic summaries (weekly, ten-day, monthly) of L2 products.
Level 4	Model output or results from analyses of lower-level data (e.g., variables derived from multiple measurements).

More on: How to compare satellite and CTMs?

- By Brasseur & Jacob (2017)
  - Model field and surface obs may not be exactly comparable
  - Averaged model field -> compare with retrieval

- Problem:
  - Retrieval makes assumption of the atmosphere (priori info) that may be inconsistent to model atm -> synthetic (shared "fake") atmosphere is needed
  - Key: what satellite would see if it's in model atmosphere, and how different is our retrieval comparing to model with same condition. That's the question.