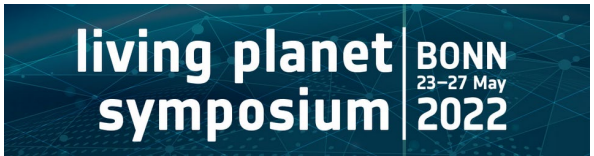
TOPAS ozone profile retrieval from TROPOMI ultraviolet spectral range in combination with CrIS infrared spectral range

Nora Mettig[1], **Mark Weber[1]**, Alexei Rozanov[1], John P. Burrows[1], Pepijn Veefkind[2]

[1] Institute of Environmental Physics (IUP), University of Bremen, Germany
[2] The Royal Netherlands Meteorological Institute (KNMI), De Bilt, Netherland



University of Bremen

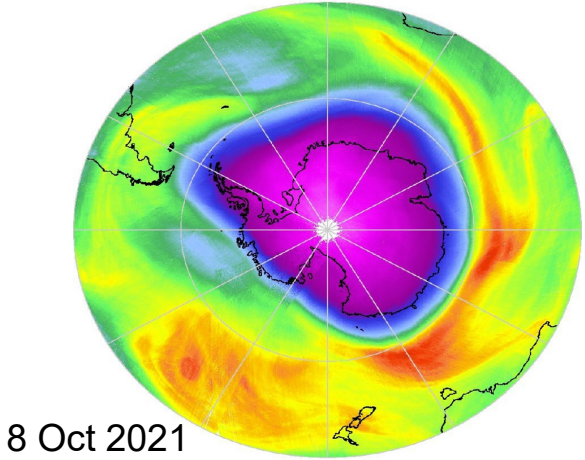
Motivation - Why do we need ozone profiles?

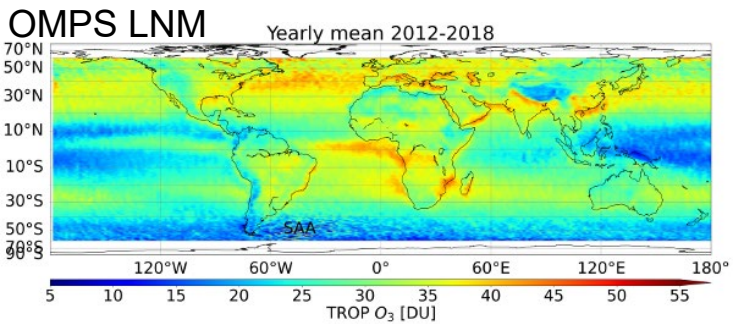
- Stratospheric ozone protects us from dangerous UV radiation
- Ozone changes in the **stratosphere** are governed by chemistry and dynamics (circulation, transport) and their relative contribution varies with altitude

→ ozone recovery (Montreal Protocol) from decreasing ozone-depleting substances and the feedback from GHG has to be monitored

- ozone in the **troposphere** is harmful for humans, plants and animals and acts as a greenhouse gas
- Sources of tropospheric ozone are chemical reactions with hydrocarbons and nitrogen oxides (man-made)

→ Tropospheric ozone content needs to be monitored for health reasons and to monitor global warming

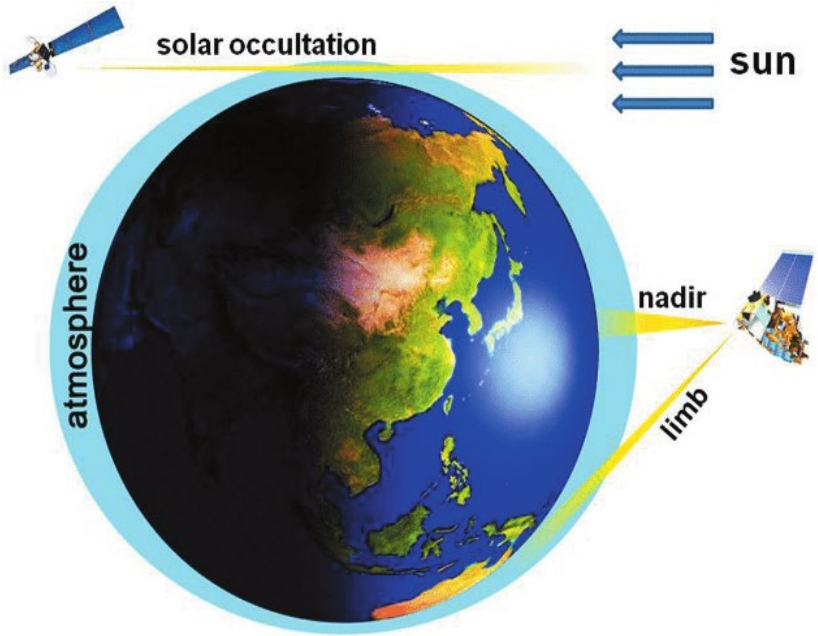




provided by Andrea Orfanoz-Cheuquelaf

University of Bremen

Motivation - why satellite based nadir measurements?



Lee et al., 2009, DOI:10.1007/978-1-4020-9674-7_2

- Nadir measurements provide information in the stratosphere **and** troposphere

BUT: nadir ozone profiles have a lower vertical resolution and contain less information about ozone than limb/occultation profiles

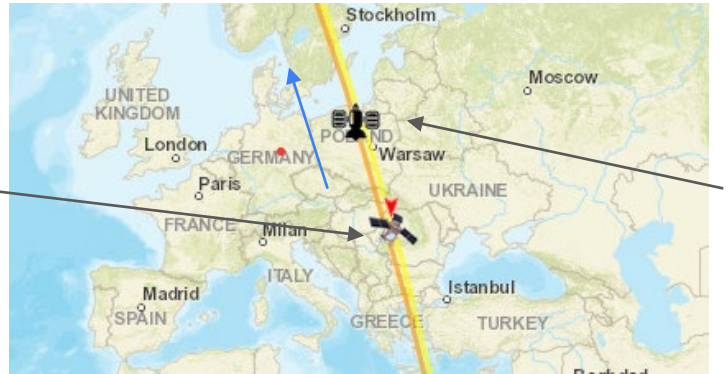
- nadir viewing instruments (UV and IR) are available in the future until 2038
  - ❑ Metop 2nd generation A1 - A3 will contain Sentinel 5 and IASI-NG

- Danger of gaps in future limb/occultation missions

University of Bremen

DATA	TROPOMI	CrIS
Platform	S5P (2018)	Suomi NPP (2011)
Used spectral range	UV1 & UV2: 270 – 329 nm	TIR: 9.35 – 9.9 µm
Spectral resolution	0.065 nm	0.625 cm^{-1} (~5 nm)
Dataset	L1B Version 2: Radiance and Irradiance	CLIMCAPS L2: cloud clear radiances and surface temperature
Spatial resolution	Spatial binning to 48x48 km or to spatial sampling from CrIS pixels	3x3 14 km FOV covering a 42x42 km cell

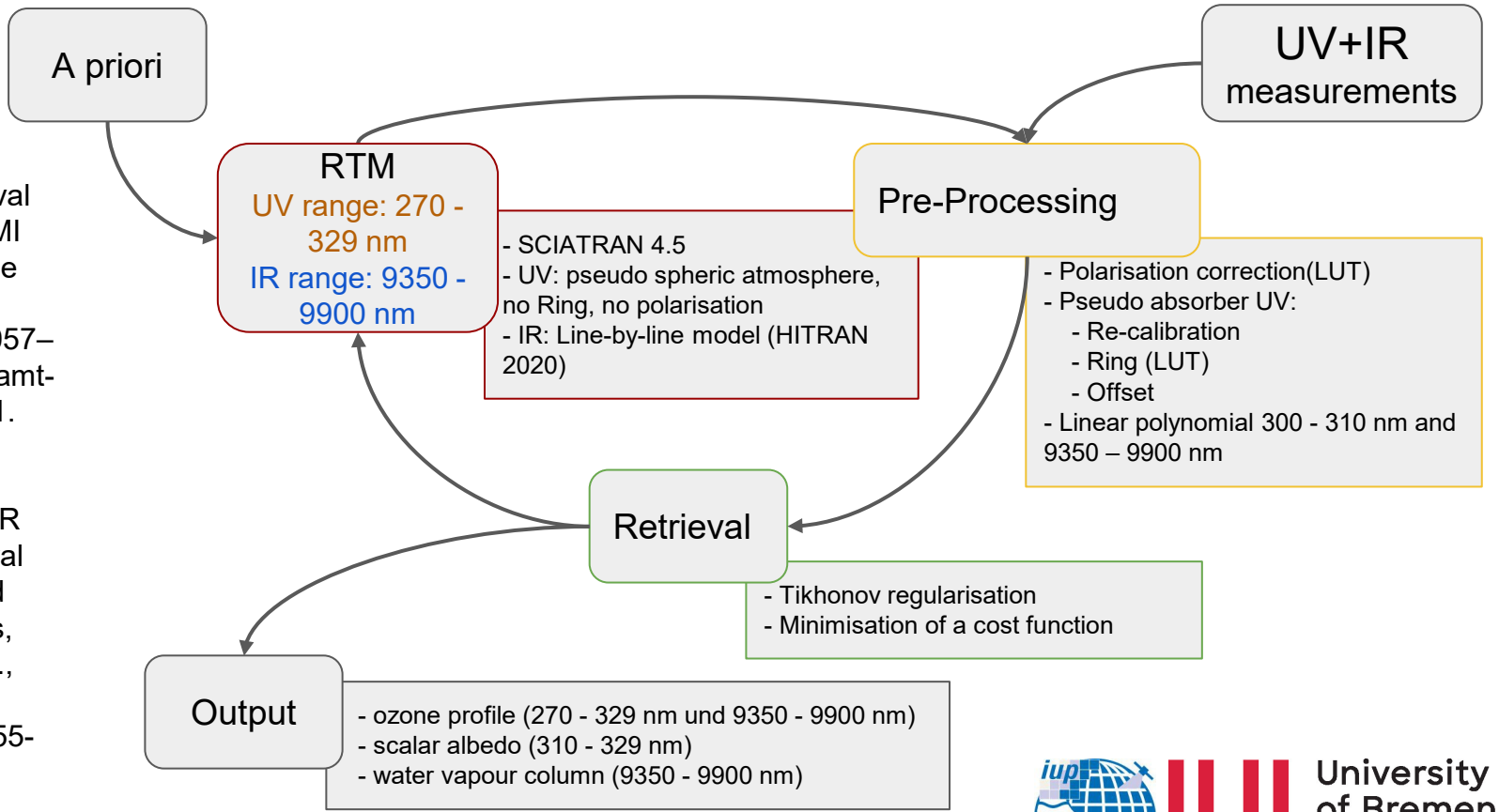
S5P



Suomi NPP (~3 minutes ahead)

University of Bremen

TOPAS - Tikhonov regularized Ozone Profile retrievAl with SCIATRAN

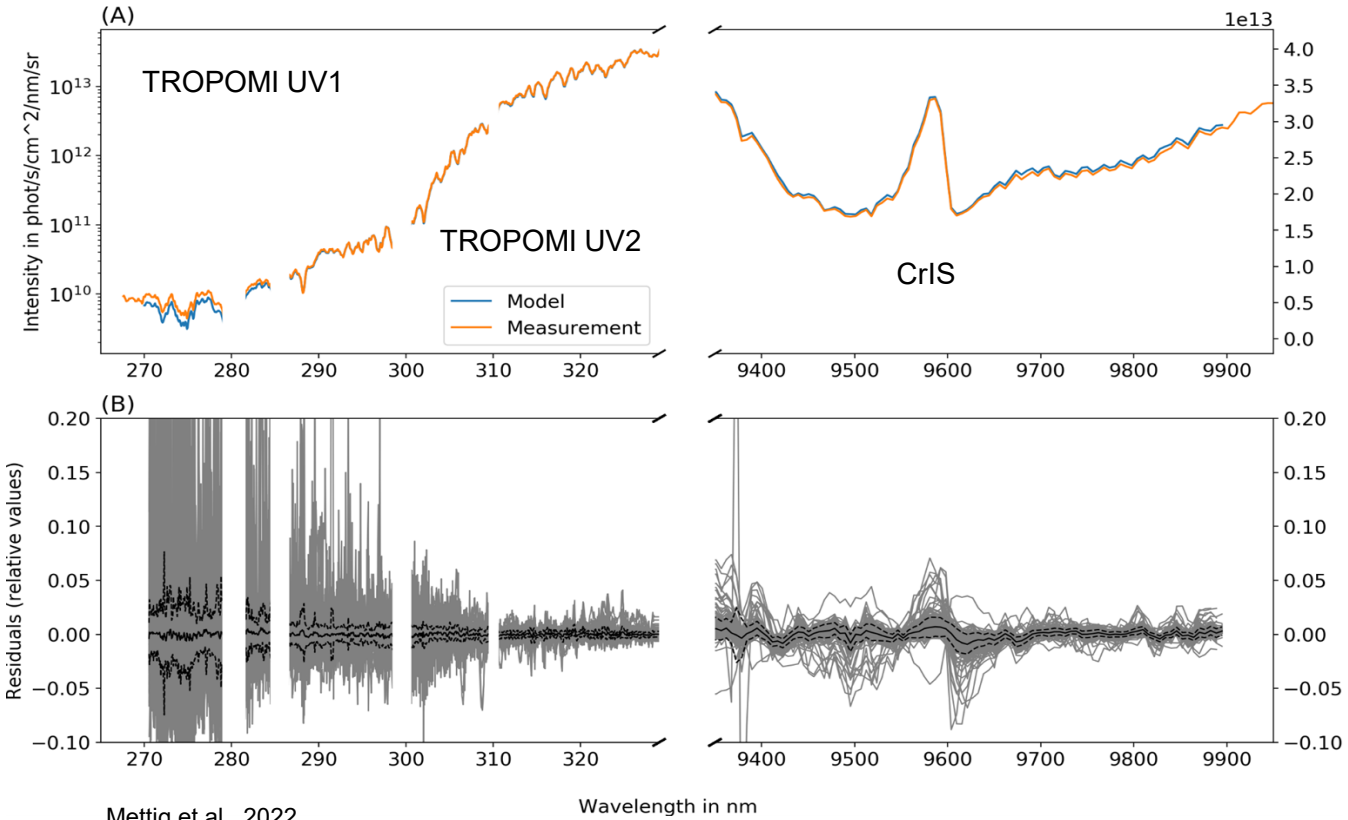


- Mettig, N., et al., Ozone profile retrieval from nadir TROPOMI measurements in the UV range, Atmos. Meas. Tech., 14, 6057–6082, doi: 10.5194/amt-14-6057-2021, 2021.

- Mettig, N., et al., Combined UV and IR ozone profile retrieval from TROPOMI and CrIS measurements, Atmos. Meas. Tech., 15, 2955–2978, doi: 10.5194/amt-15-2955-2022, 2022.

University of Bremen

Example of measured and modelled spectra



Mettig et al., 2022

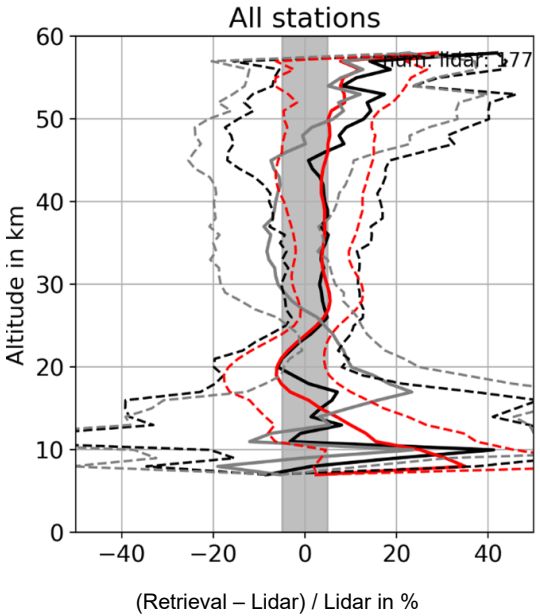
Example TROPOMI/CrIS Pixel on 6 July 2018 after 1st iteration

Residuals of around 300 TROPOMI/CrIS Pixel with collocated ozone sonde profiles available (used for validation)

University of Bremen

TROPOMI UV Retrieval validation

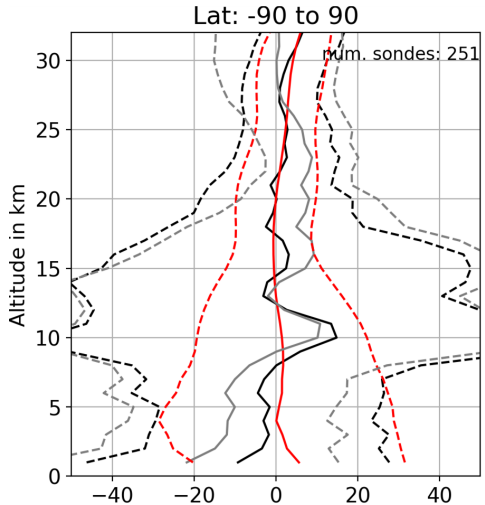
Stratospheric Lidar



Validation with 177 collocated stratospheric lidar profiles from 5 sites

– retrieval – lidar
– retrieval – lidar x AK
– a priori – lidar

Ozone sondes



Validation with 251 collocated ozone sonde profiles from 26 sites

– retrieval – sonde
– retrieval – sonde x AK
– a priori – sonde

Mettig et al., 2021

University of Bremen

Combined UV and IR retrieval characteristics

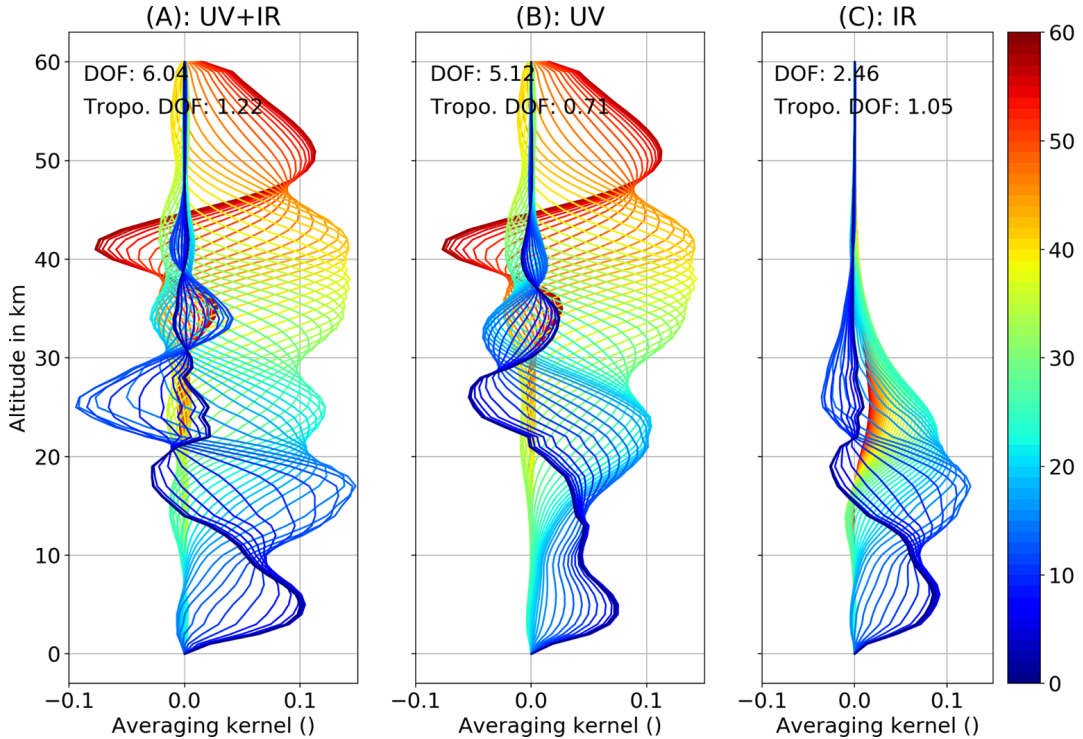
Combined retrieval advantage:

- stratospheric ozone profile mainly based on TROPOMI UV measurements
- improved tropospheric ozone information by using additional IR spectra

→ increase of ~1 DOF

→ less than other studies with TES or IASI (Worden et al. 2007, Fu et al. 2013, Cuesta et al., 2013)

→ CrIS's spectral resolution is lower

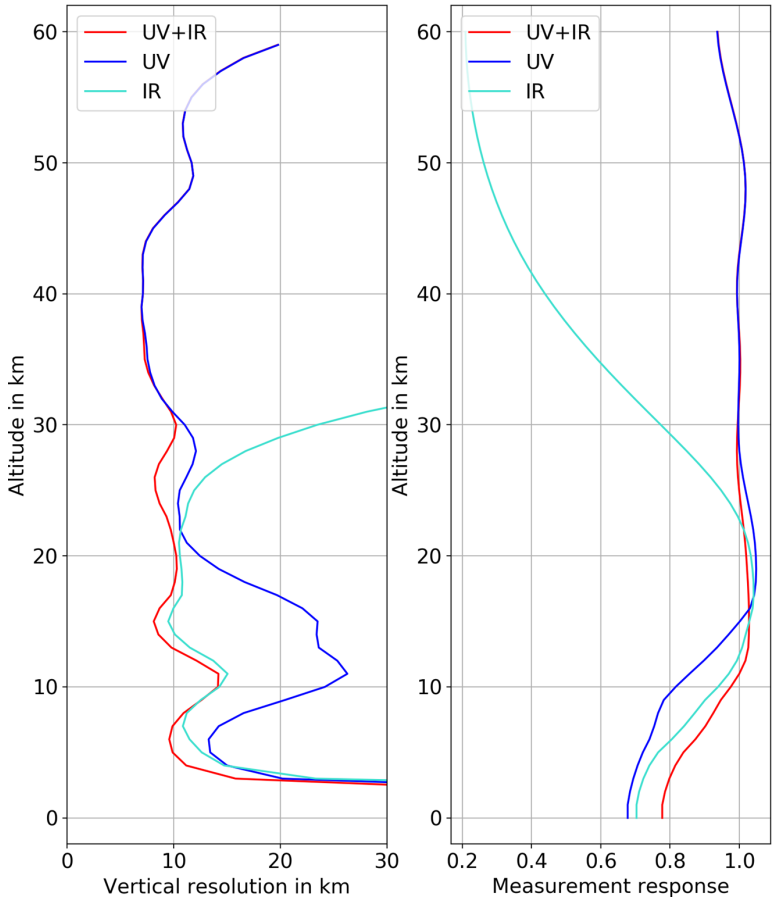


Note: UV only and IR only use settings from the optimised UV+IR retrieval (not the optimum of the individual settings)

Mettig et al., 2022

University of Bremen

Combined ozone profile retrieval example



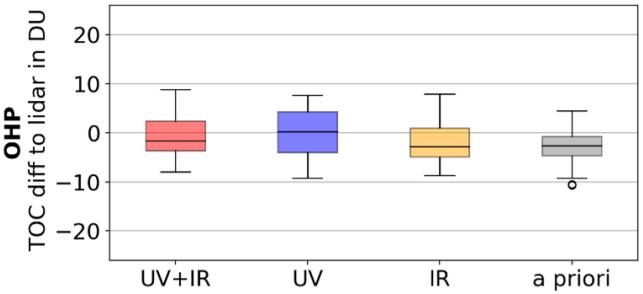
- vertical resolution: inverse of AK diaginal elements
- measurement response: sum of the AK rows

→ improved vertical resolution and measurement response in the troposphere

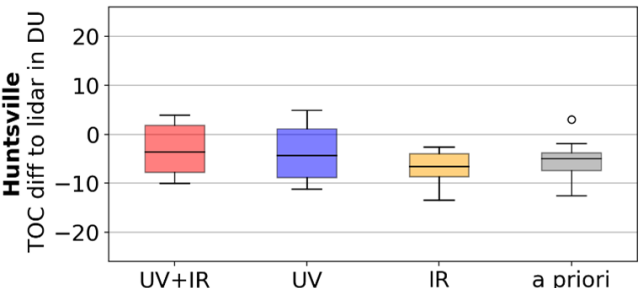
→ no impact of IR measurements in the stratosphere above 30 km

University of Bremen

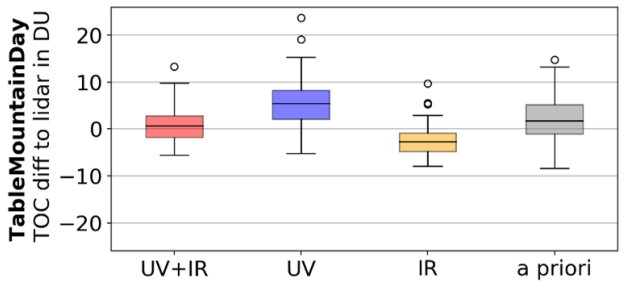
Combined retrieval validation - tropospheric ozone columns (TOC)



- A priori: -3.0DU ±3.8DU (1σ)
- IR: -1.7DU ±4.1DU (1σ)
- UV: -0.2DU ±4.9DU (1σ)
- UV+IR: -0.8DU ±3.9DU (1σ)



- A priori: -5.6DU ±4.0DU (1σ)
- IR: -6.8DU ±3.2DU (1σ)
- UV: -3.7DU ±5.5DU (1σ)
- UV+IR: -3.1DU ±4.8DU (1σ)



- A priori: 2.6DU ±4.8DU (1σ)
- IR: -2.3DU ±3.5DU (1σ)
- UV: 5.7DU ±5.8DU (1σ)
- UV+IR: 0.7DU ±3.9DU (1σ)

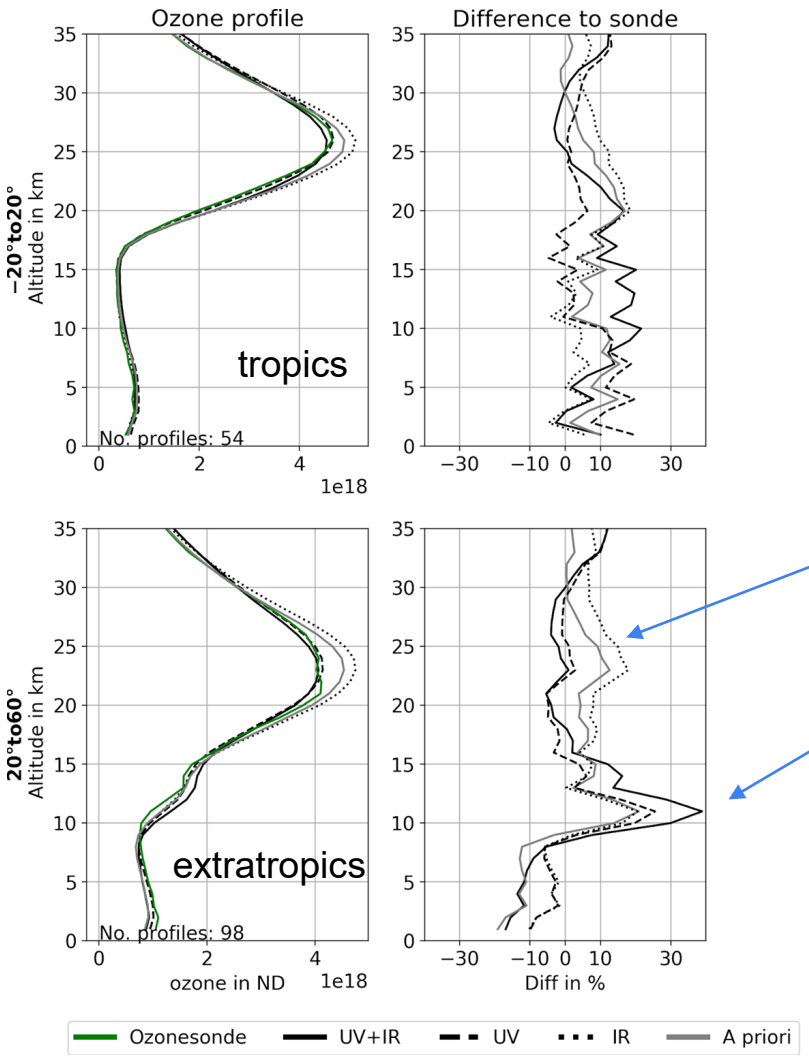
validation data: ground-based tropospheric lidars from 3 sites

→ combined retrieval bias and scatter is generally lower

Mettig et al., 2022

University of Bremen

Issues with combined retrieval



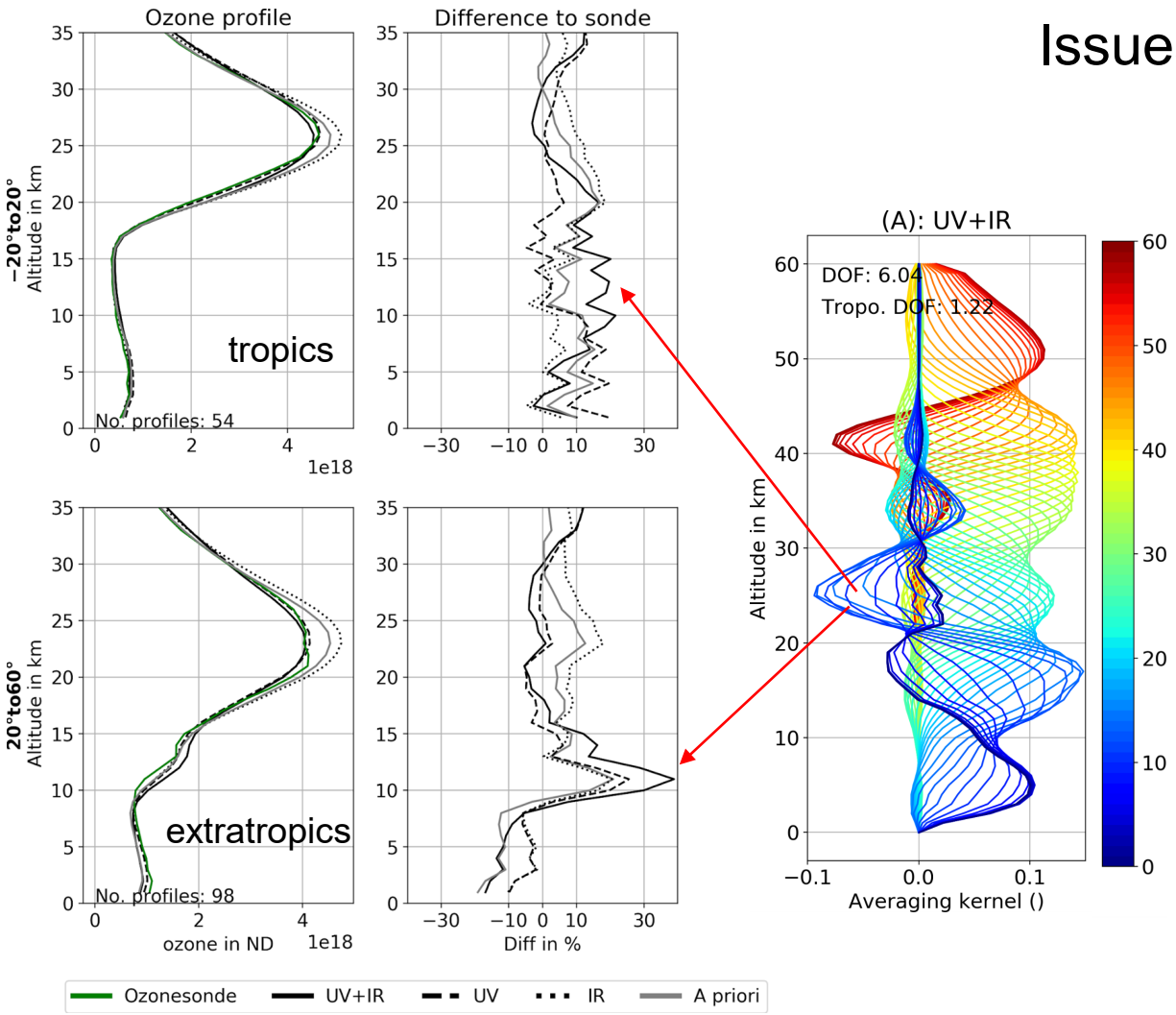
comparison with ozone sonde profiles

- IR retrieval: positive bias between 15 – 30 km
- combined retrieval: positive bias between 10 – 15 km

→ stratospheric IR bias is shifted downwards in the combined retrieval

University of Bremen

Issues with combined retrieval



comparison with ozone sonde profiles

- IR retrieval: positive bias between 15 – 30 km
- combined retrieval: positive bias between 10 – 15 km

→ stratospheric IR bias is shifted downwards in the combined retrieval

University of Bremen

Conclusion

- A new and improved re-calibration approach (Mettig et al., 2021) allows to retrieve ozone profiles from TROPOMI L1B measurements with very good agreement with MLS, OMPS, lidars and ozone sondes in the stratosphere, but tropospheric ozone information is limited
- TOPAS retrieval allows combining TROPOMI UV and CrIS IR measurements (Mettig et al. 2022)
  - improved information content by ~1 DOF
  - tropospheric ozone columns from UV+IR have lower bias and standard deviation compared to single spectral range retrievals
- Ozone profiles from UV+IR show a positive bias in the 10-15km altitude range, which has to be further investigated

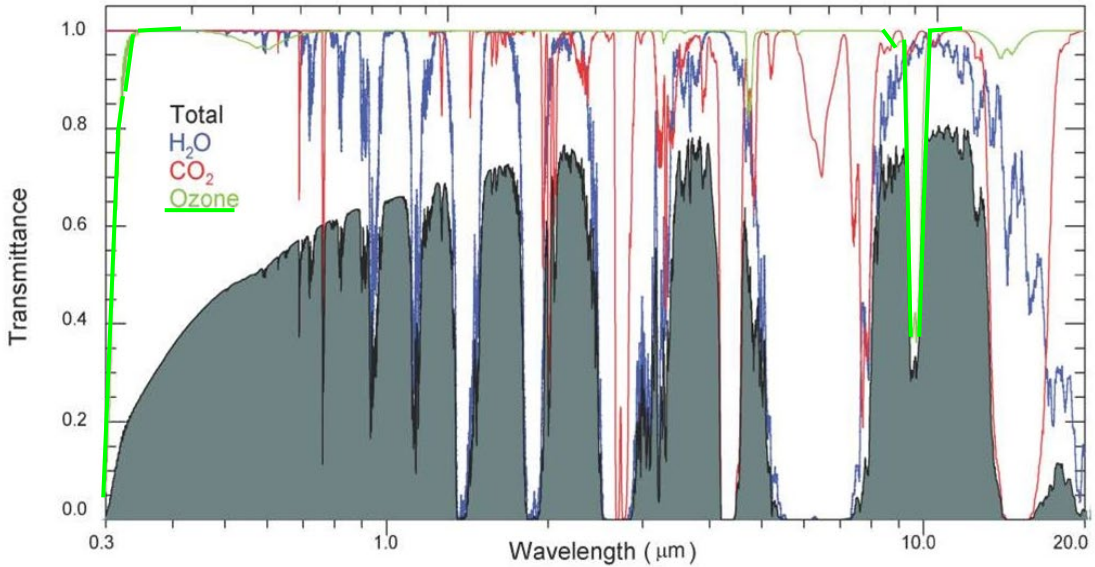
Thank you for your attention!

University of Bremen

Motivation - Ozone profiles from UV and IR spectrum

Ozone absorbs radiation in the:

- **ultraviolet (UV)**
- visible (VIS)
- **thermal infrared (IR)** and
- microwave spectra



http://what-when-how.com/remote-sensing-from-air-and-space/atmospheric-absorption-scattering-and-turbulence-visible-imagery-remote-sensing/

Ozone profile information comes from:

- UV: wavelength dependent penetration depth of the incoming radiation
- IR: decreasing atmospheric density with height

not enough information about tropospheric ozone

UV re-calibration using simulations with MLS ozone profiles

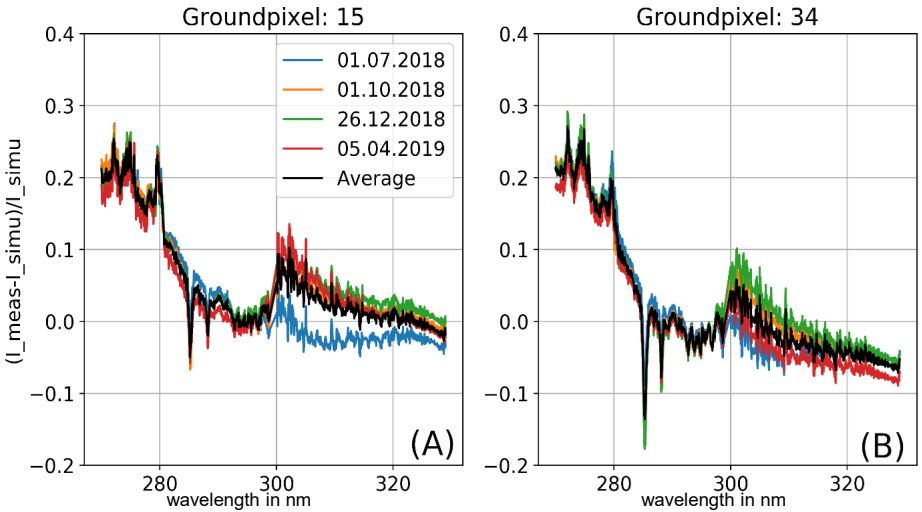
- For cloudfree pixels in tropics and extratropics: simulating intensities using MLS ozone profiles and pixel properties (Liu et al., 2010)

- **new approach (Mettig et al., 2021)**:

  correction spectra treated as pseudo absorber → flexible amplitude and wavelength grid → deal with uncertainties and time dependence

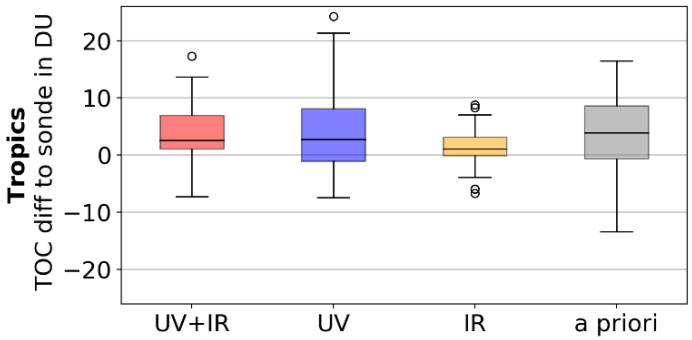
  Corrections due to Rayleigh scattering above 60 km is included in the re-calibration → allows reducing the top altitude of retrieval grid down to 60 km halving the computing time

$$Factor_{corr}(\lambda) = \frac{I_{meas}(\lambda) - I_{simu}(\lambda)}{I_{simu}(\lambda)}$$

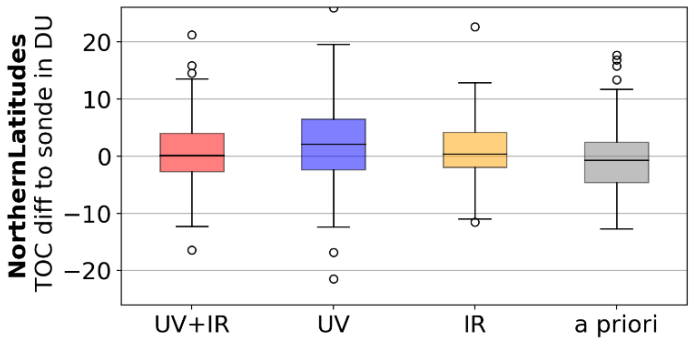


Mettig et al., 2021

Combined retrieval validation - tropospheric ozone columns (TOC)



- A priori: 3.0 DU ±6.8 DU (1σ)
- IR: 1.3 DU ±3.2 DU (1σ)
- UV: 3.7 DU ±6.4 DU (1σ)
- UV+IR: 3.8 DU ±4.9 DU (1σ)



- A priori: -0.4 DU ±5.7 DU (1σ)
- IR: 1.0 DU ±5.1 DU (1σ)
- UV: 2.1 DU ±7.3 DU (1σ)
- UV+IR: 0.6 DU ±5.8 DU (1σ)

validation data: ozone sonde profiles in the tropics (-20° – 20°) and northern latitudes (30° – 60°)

- combined retrieval bias and/or scattering is lower

Mettig et al., 2022