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Harmonization of tropospheric ozone data records from satellites

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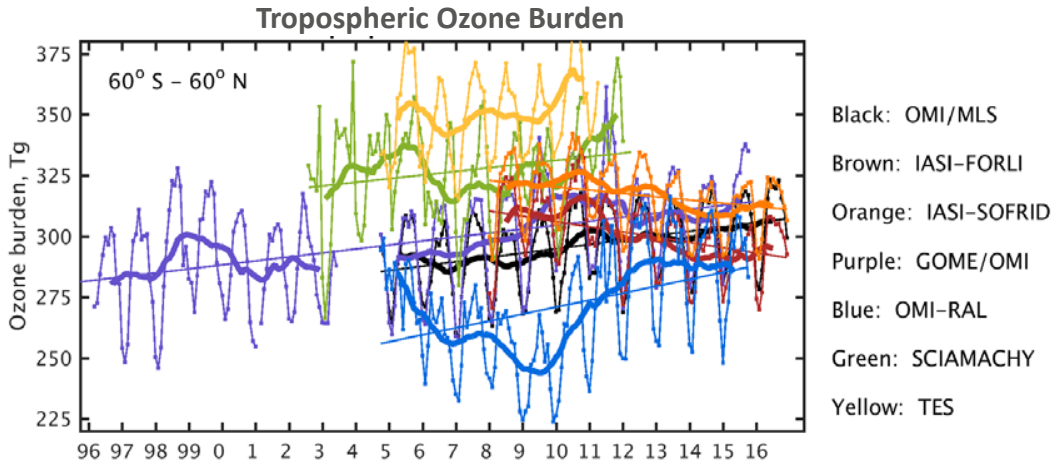
Royal Belgian Institute for Space Aeronomy

CEOS VC-20-01 rationale

"Tropospheric ozone dataset validation and harmonization" in response to

TOAR-II Satellite Ozone WG needs, addressing

- wide range of tropospheric ozone levels and trends from satellites
- differences in vertical sensitivity, sampling, and vertical range
- changes in bias over time



(TOAR-I, Gaudel, et al., 2018)

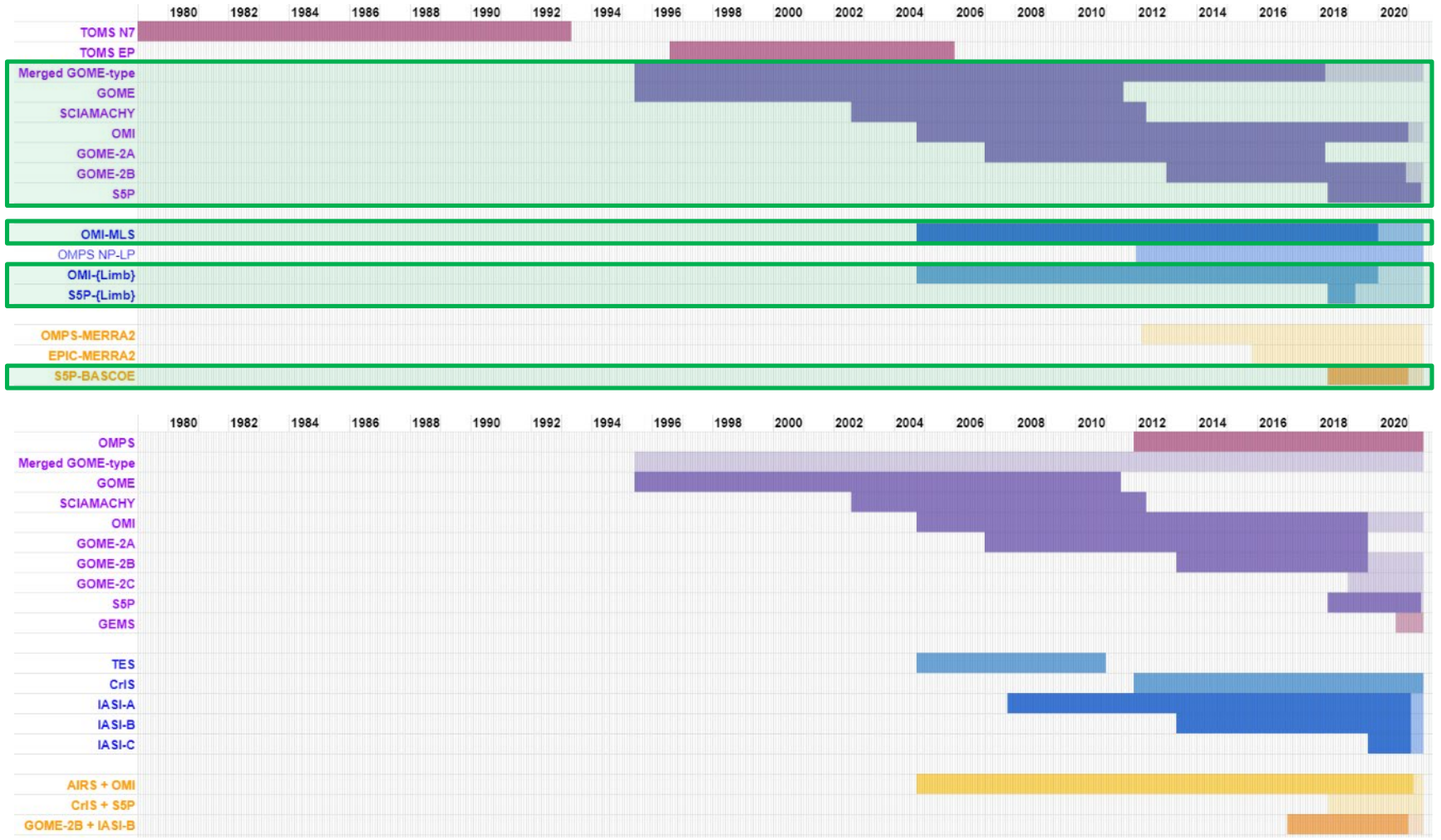
by application of

- satellite data harmonization
- harmonized validation process to identify and quantify remaining discrepancies

Transfer standard: CAMS Reanalysis EAC4

- CAMSRA (Inness *et al.*, 2019)
  - 60 levels (1012-0.1 hPa) → lat-lon dependent, fixed in time
  - 0.7° x 0.7° (global) → regridded to 1° x 1°
  - 6 hours (2003-2021) → UTC interpolated to LST satellite overpass time
  - assimilated ozone: TC (SCIA, OMI, GOME-2A/B), PROF (MIPAS, Aura-MLS, SBUV/2)
- Used for
  - tropospheric column extension
  - new prior info
  - auxiliary data source for quantity matching
  - (assessment of horizontal and temporal sampling differences)
- Complementary choice to TCR-2 reanalysis (Miyazaki *et al.*, 2020) transfer standard used by TOAR-II SOWG

VC-20-01 tropospheric ozone datasets



Residual technique (UV-VIS sensors)

- Convective Cloud Differential
- Nadir minus Limb
- Nadir minus Reanalysis

Optimal Estimation profile retrieval

- UV-VIS
- IR
- VIS+IR synergy

Harmonization of tropospheric column data

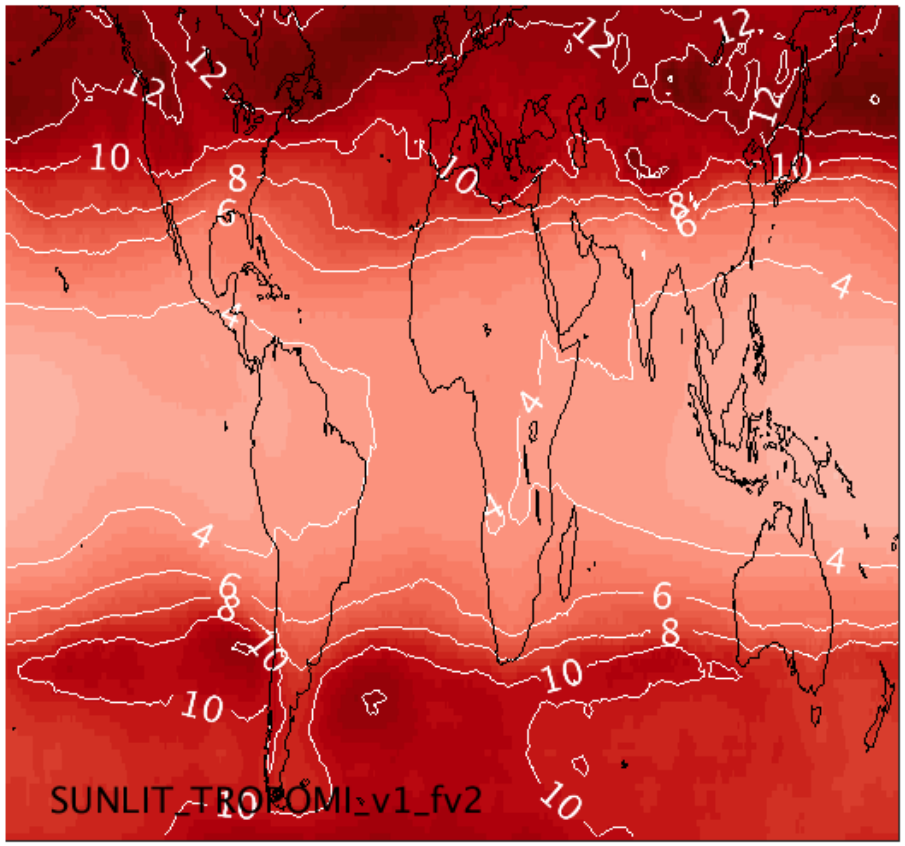
- Different data records have different Top of Troposphere definition l
  - CCD DLR : fixed pressure 270 hPa
  - CCD IUP : fixed pressure 200 hPa
  - SUNLIT : altitude WMO lapse-rate tropopause – 3 km (ERA5)
  - S5P-BASCOE : pressure dynamical tropopause (ERA5)
  - OMI-MLS : pressure WMO lapse-rate tropopause (NCEP)
- Harmonization equation (top level $l \rightarrow l'$):

$$X(\mathrm{sfc}, l') = X(\mathrm{sfc}, l\,) + \int_{\mathrm{sfc}}^{l'} x_{CAMSRA}(p)dp - \int_{\mathrm{sfc}}^{l} x_{CAMSRA}(p)dp$$

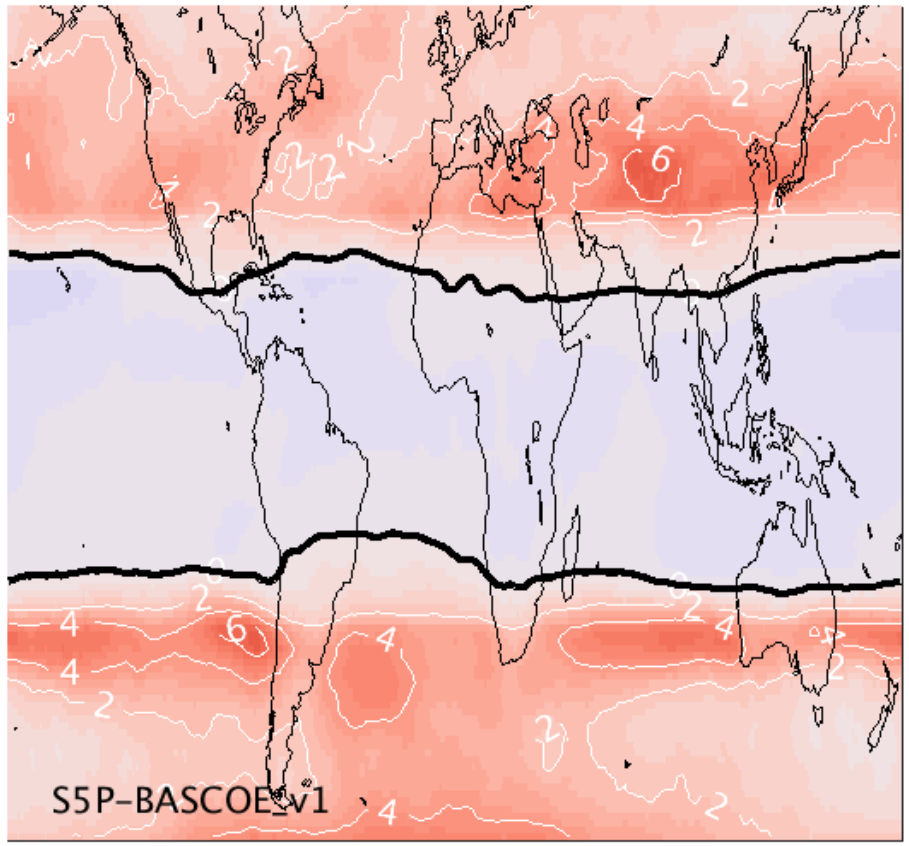
- Challenges:
  - Not reported in data files: tropospheric top level, geolocation input data
  - Harmonized monthly mean data ≠ monthly mean of harmonized daily data
  - Correct for mean bias between $X(\mathrm{sfc}, l)$ and $X_{CAMSRA}(\mathrm{sfc}, l)$? How?

Illustration: native ToTr level → LRT_{NCEP}

TrOC(LRT_{NCEP}) – TrOC(LRT-3km)



TrOC(LRT_{NCEP}) – TrOC(dyn TP)

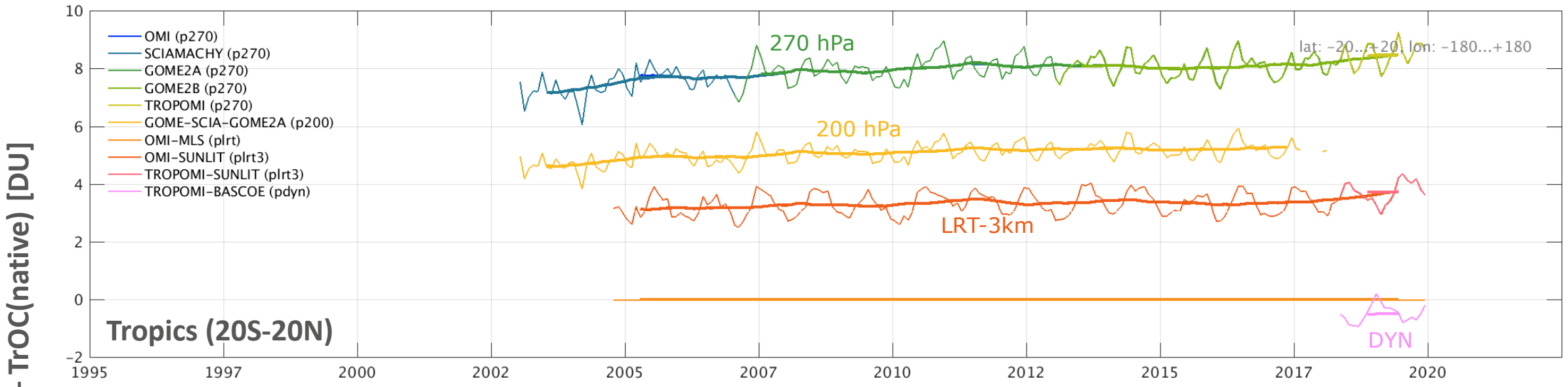


Temporal mean (2019) harmonization term

Clear impact on spatial distribution due to varying top level definition.

- LRT_{NCEP} : OMI-MLS
- LRT-3km : SUNLIT
- dyn. TP : S5P-BASCOE

Illustration: native ToTr level → LRT_{NCEP}



Spatial mean harmonization term

Some impact on long-term changes, due to varying ToTr level definition.

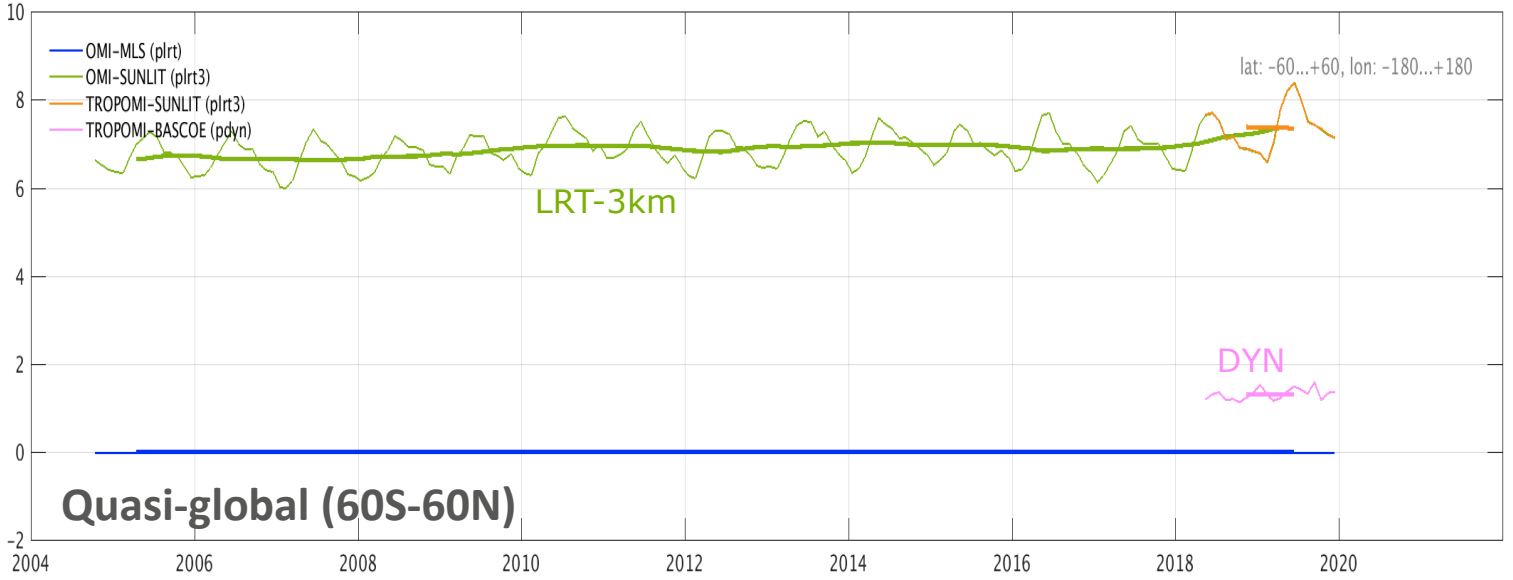
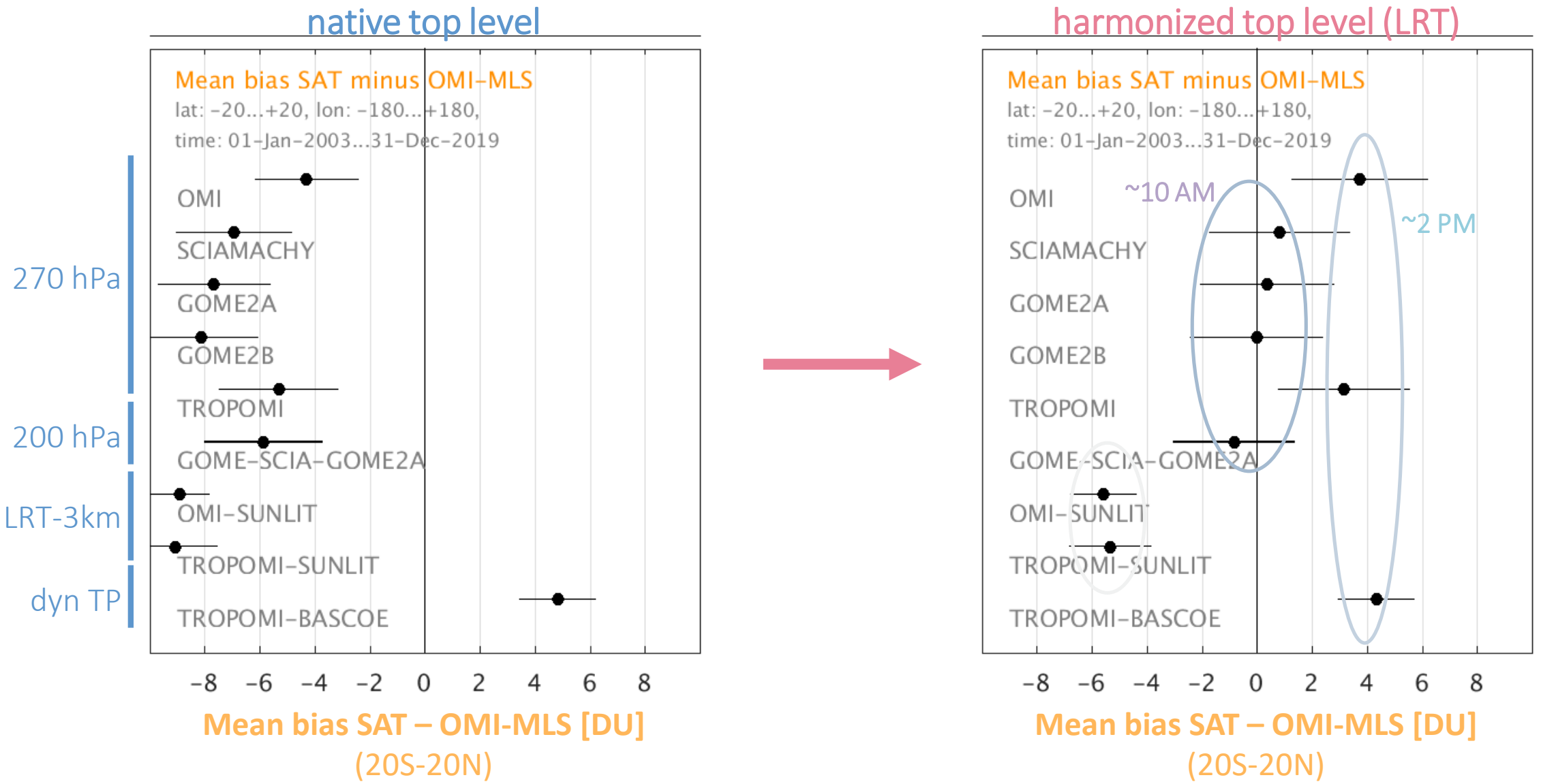
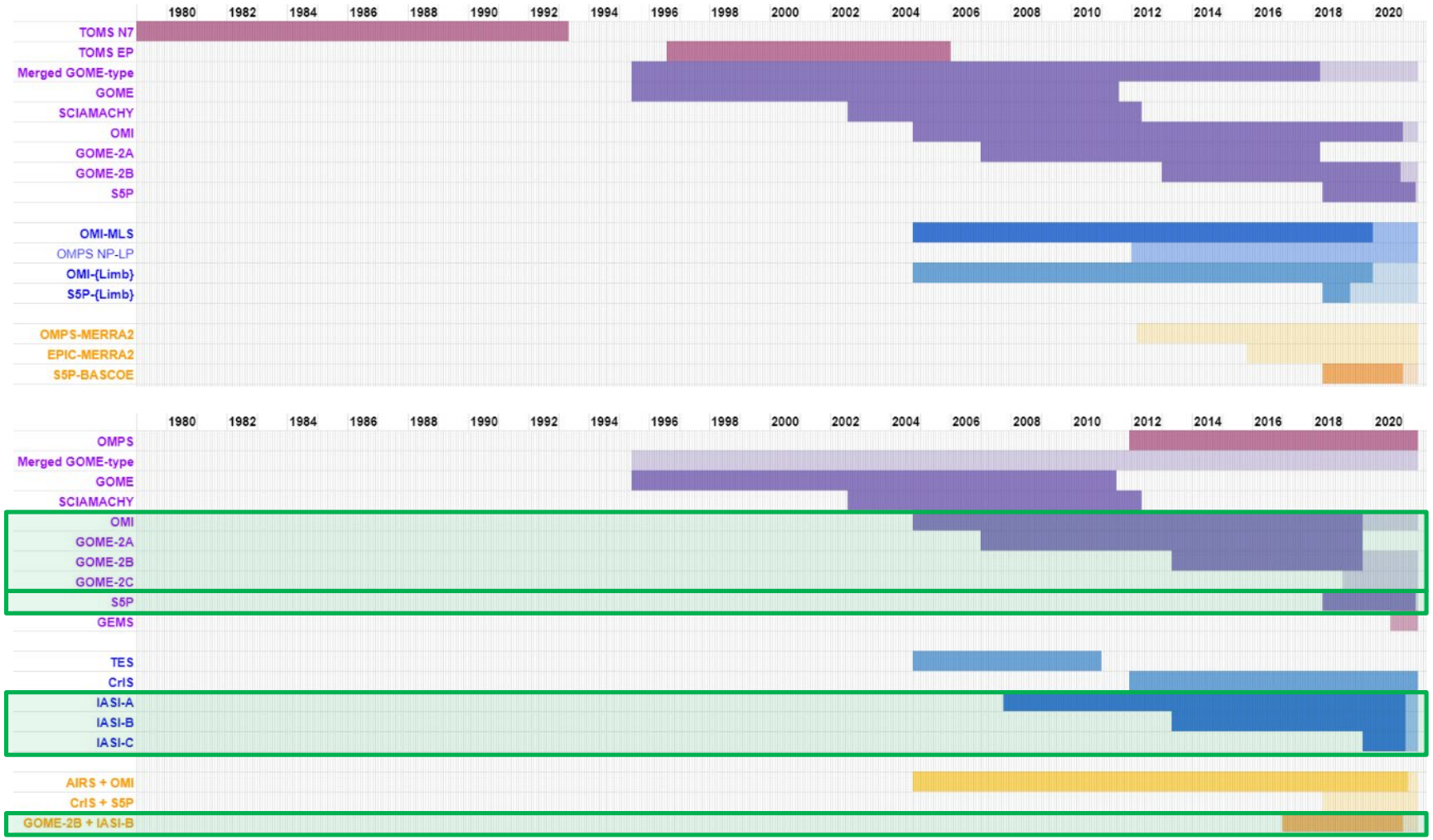


Illustration: native ToTr level → LRT_{NCEP}



VC-20-01 tropospheric ozone datasets



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Atmospheric Measurement Techniques
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Harmonization and comparison of vertically resolved atmospheric state observations: methods, effects, and uncertainty budget

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remote sensing

MDPI

Technical Note

Removing Prior Information from Remotely Sensed Atmospheric Profiles by Wiener Deconvolution Based on the Complete Data Fusion Framework

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Harmonization for a single profile retrieval

Matching operation	$\boldsymbol{x}'$	$\mathbf{S}'$	$\mathbf{A}'$
Vert. quantity matching	$\mathbf{M}\boldsymbol{x}$	$\mathbf{M}\mathbf{S}\mathbf{M}^T$	$\mathbf{M}\mathbf{A}\mathbf{M}^{-1}$
Vert. sampling matching	$\mathbf{W}\boldsymbol{x}$	$\mathbf{W}\mathbf{S}\mathbf{W}^T$	$\mathbf{W}\mathbf{A}\mathbf{W}^*$
Vert. smoothing matching	$\mathbf{V}\boldsymbol{x}$	$\mathbf{V}\mathbf{S}\mathbf{V}^T$	$\mathbf{V}\mathbf{A}$
Meas. weight matching	$\mathbf{W}^{\mathrm{M}}\boldsymbol{x}$	$\mathbf{S}$	$\mathbf{W}^{\mathrm{M}}\mathbf{A}$
Prior matching (PM)	$\mathbf{S}'(\mathbf{S}^{-1}\boldsymbol{x} - \mathbf{R}_a\boldsymbol{x}_a + \mathbf{R}'_a\boldsymbol{x}'_a)$	$(\mathbf{S}^{-1} - \mathbf{R}_a + \mathbf{R}'_a)^{-1}$	$\mathbf{A} + \mathbf{S}\mathbf{S}_a^{-1} - \mathbf{S}'\mathbf{S}'^{-1}_a$
Re-optimized PM	$\mathbf{P}[\boldsymbol{x} - (\mathbf{I} - \mathbf{A})\boldsymbol{x}_a] + \mathbf{P}\mathbf{S}(\mathbf{A}^T)^{-1}\mathbf{R}'_a\boldsymbol{x}'_a$	$\mathbf{P}\mathbf{S}\mathbf{P}^T$	$\mathbf{P}\mathbf{A}$
AK smoothing (for s on r)	$\mathbf{A}_{\mathrm{s}}\boldsymbol{x}_{\mathrm{r}} + (\mathbf{I} - \mathbf{A}_{\mathrm{s}})\boldsymbol{x}_{\mathrm{a,s}}$	$\mathbf{A}^1_{\mathrm{s}}\mathbf{S}_{\mathrm{r}}(\mathbf{A}^1_{\mathrm{s}})^T$	$\mathbf{A}_{\mathrm{s}}$
Maximum likelihood repr.	$\mathbf{S}'(\mathbf{S}^{-1}\boldsymbol{x} - \mathbf{R}_a\boldsymbol{x}_a)$	$(\mathbf{S}^{-1} - \mathbf{R}_a)^{-1}$	$\mathbf{I}$
Information-centered repr.	$\mathbf{W}(\mathbf{S}^{-1} - \mathbf{R}_a)^{-1}(\mathbf{S}^{-1}\boldsymbol{x} - \mathbf{R}_a\boldsymbol{x}_a)$	$\mathbf{W}(\mathbf{S}^{-1} - \mathbf{R}_a)^{-1}\mathbf{W}^T$	$\mathbf{I}'$
Co-location matching	$\boldsymbol{x} - \boldsymbol{\Delta m}$	$\mathbf{S} + \mathbf{S}_{\Delta m}$	$\mathbf{A} - \mathbf{S}_{\Delta m}\mathbf{S}_a^{-1}$

(Keppens, et al., 2019)

Based on Complete Data Fusion (CDF) framework

CDF (Ceccherini et al., 2022):

$$x'_N = \left(\sum_{i=1}^{N} S_i^{-1} A_i + S_a'^{-1} \right)^{-1} \left(\sum_{i=1}^{N} S_i^{-1} [x_i - (I - A_i) x_{a,i}] + S_a'^{-1} x'_a \right)$$

where the sum is taken over N profiles within a predefined spatiotemporal domain

The corresponding averaging kernel matrix and covariance matrix are given by

$$A'_N = \left(\sum_{i=1}^{N} S_i^{-1} A_i + S_a'^{-1} \right)^{-1} \left(\sum_{i=1}^{N} S_i^{-1} A_i \right)$$

and

$$S'_N = \left(\sum_{i=1}^{N} S_i^{-1} A_i + S_a'^{-1} \right)^{-1}$$

which is mathematically equivalent to a joint retrieval (Ceccherini et al., 2015)

Choice of new prior info determines CDF output

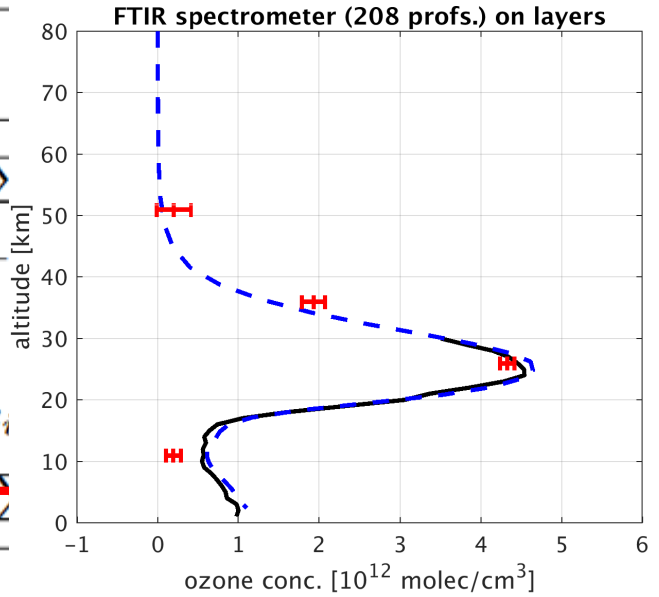
Abbr.	x'_a	S'^{-1}_a	x'_N	
CDF	x_m	αS_m^{-1}	$\left(\sum S_i^{-1} A_i + \alpha S_m^{-1}\right)^{-1} \left(\sum S_i^{-1} [x_i - (I - A_i) x_{a,i}] + \alpha S_m^{-1} x_m\right)$	~ MLR if α = 0
APR	x_m	$\sum S_{a,i}^{-1}$	$\left(\sum S_i^{-1}\right)^{-1} \left(\sum S_i^{-1} [x_i - (I - A_i)(x_{a,i} - x_m)]\right)$	
WAV	$x_{a,i}$	$\sum S_{a,i}^{-1}$	$\left(\sum S_i^{-1}\right)^{-1} \left(\sum S_i^{-1} x_i\right)$	
MLR	$x_{a,i}$	0	$\left(\sum S_i^{-1} A_i\right)^{-1} \left(\sum S_i^{-1} [x_i - (I - A_i) x_{a,i}]\right)$	~ deconv. on original grid
ICR*	0	0	$\left(\sum W_i^{*T} S_i^{-1} A_i W_i^*\right)^{-1} \left(\sum W_i^{*T} S_i^{-1} [x_i - (I - A_i) x_{a,i}]\right)$	~ deconv. on DFS grid

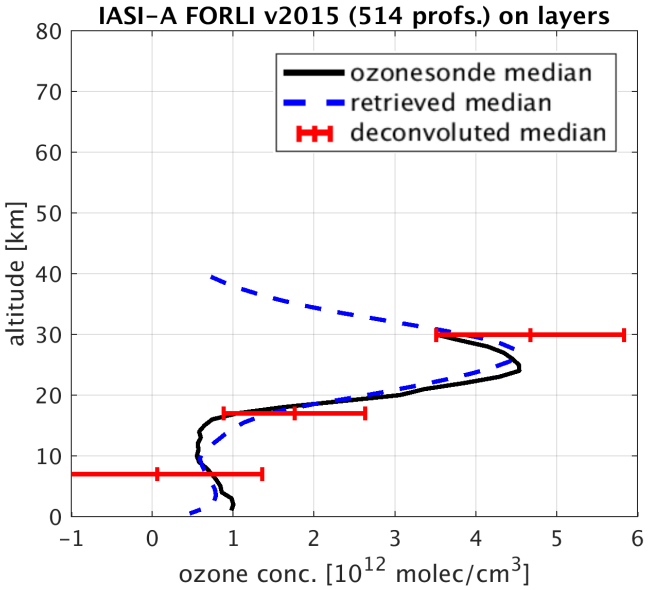
Abbr.	x'_a	S'^{-1}_a	A'_N	S'_N
CDF	x_m	αS_m^{-1}	$\left(\sum S_i^{-1} A_i + \alpha S_m^{-1}\right)^{-1} \left(\sum S_i^{-1} A_i\right)$	$\left(\sum S_i^{-1} A_i + \alpha S_m^{-1}\right)^{-1}$
APR	x_m	$\sum S_{a,i}^{-1}$	$\left(\sum S_i^{-1}\right)^{-1} \left(\sum S_i^{-1} A_i\right)$	$\left(\sum S_i^{-1}\right)^{-1}$
WAV	$x_{a,i}$	$\sum S_{a,i}^{-1}$	$\left(\sum S_i^{-1}\right)^{-1} \left(\sum S_i^{-1} A_i\right)$	$\left(\sum S_i^{-1}\right)^{-1}$
MLR	$x_{a,i}$	0	I	$\left(\sum S_i^{-1} A_i\right)^{-1}$
ICR*	0	0	$I' = W_i W_i^*$ $(\forall i)$	$\left(\sum W_i^{*T} S_i^{-1} A_i W_i^*\right)^{-1}$

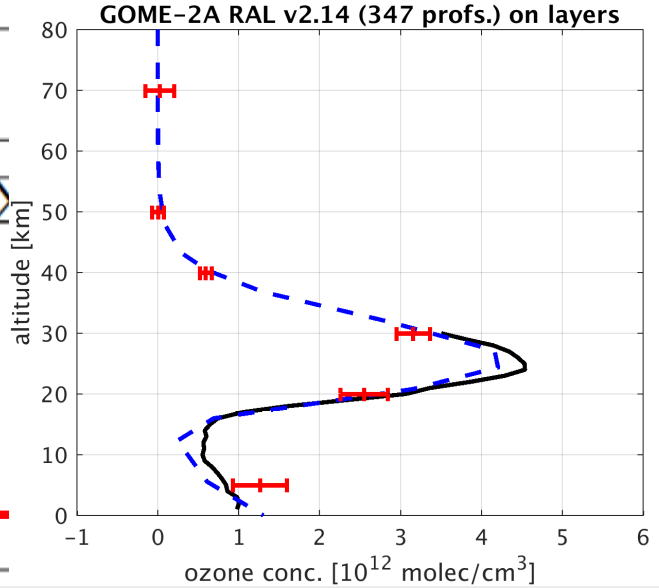
Choice of new prior info determines CDF output

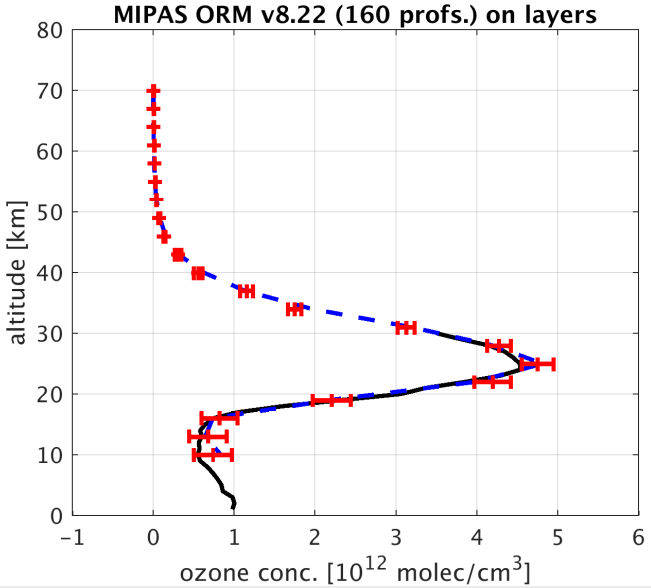
Abbr.	x'_a	S'^{-1}_a	x'_N
CDF	x_m	αS_m^{-1}	$\left(\sum S_i^{-1}A_i + \alpha S_m^{-1}\right)^{-1}\left(\sum$
APR	x_m	$\sum S_{a,i}^{-1}$	$\left(\sum S_i^{-1}\right)^{-1}\left(\sum S_i^{-1}[x_i -\right.$
WAV	$x_{a,i}$	$\sum S_{a,i}^{-1}$	$\left(\sum S_i^{-1}\right)^{-1}\left(\sum S_i^{-1}x_i\right)$
MLR	$x_{a,i}$	0	$\left(\sum S_i^{-1}A_i\right)^{-1}\left(\sum S_i^{-1}[x_i\right.$
ICR*	0	0	$\left(\sum W_i^{*T}S_i^{-1}A_iW_i^*\right)^{-1}\left(\sum\right.$

Abbr.	x'_a	S'^{-1}_a	A'_N
CDF	x_m	αS_m^{-1}	$\left(\sum S_i^{-1}A_i + \alpha S_m^{-1}\right)^{-1}\left(\sum\right.$
APR	x_m	$\sum S_{a,i}^{-1}$	$\left(\sum S_i^{-1}\right)^{-1}\left(\sum S_i^{-1}A_i\right)$
WAV	$x_{a,i}$	$\sum S_{a,i}^{-1}$	$\left(\sum S_i^{-1}\right)^{-1}\left(\sum S_i^{-1}A_i\right)$
MLR	$x_{a,i}$	0	I
ICR*	0	0	$I' = W_iW_i^* \ (\forall i)$









Harmonization of TOAR-II profile datasets

- L2 profiles → monthly-gridded (1°x1°) & harmonized (prior info) satellite L3 data
- Illustration: 1° x 1° box containing Brussels, for January 2020
- Comparison with both CAMSRA and Uccle ozonesondes
- Sampling example: March 24, 2021 (courtesy of N. Zoppetti, IFAC)

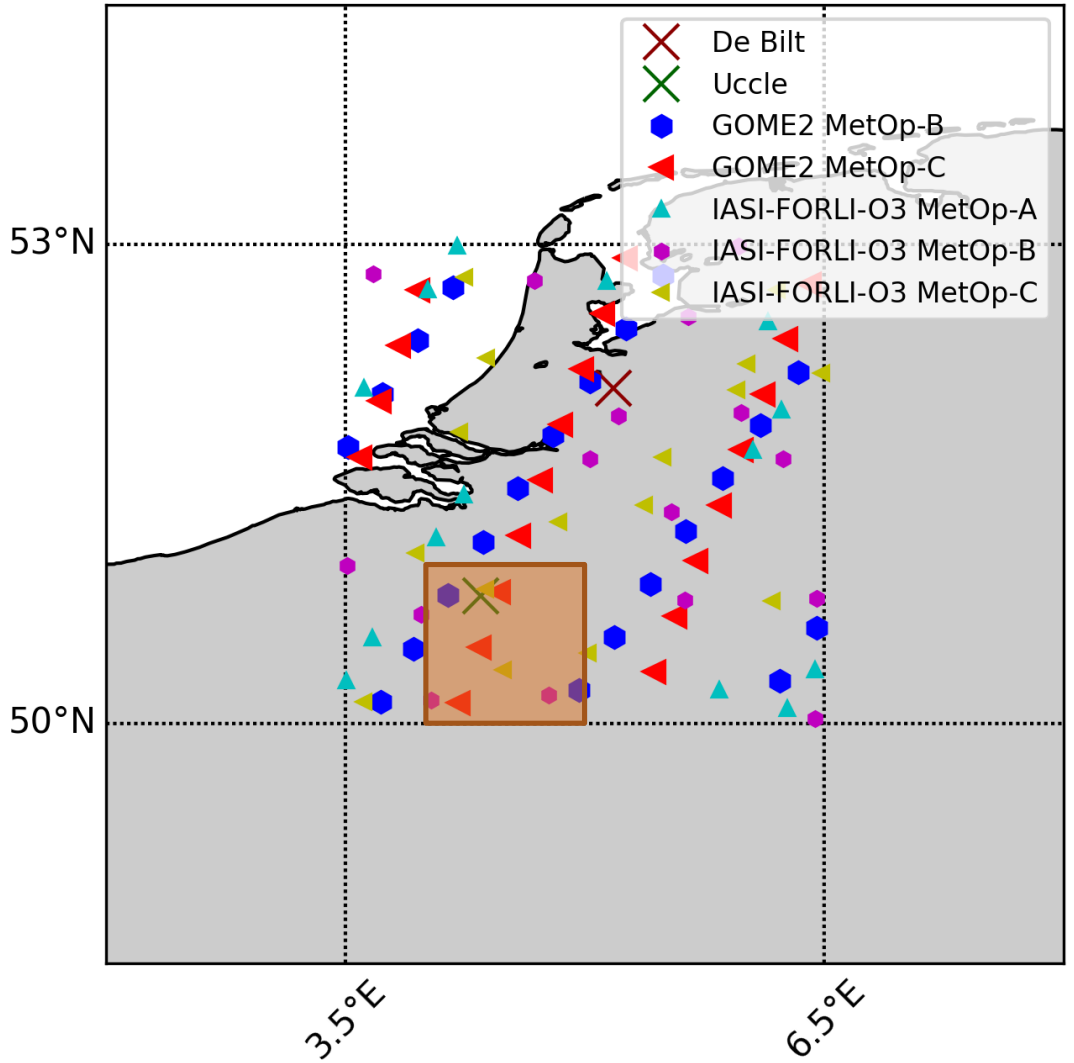
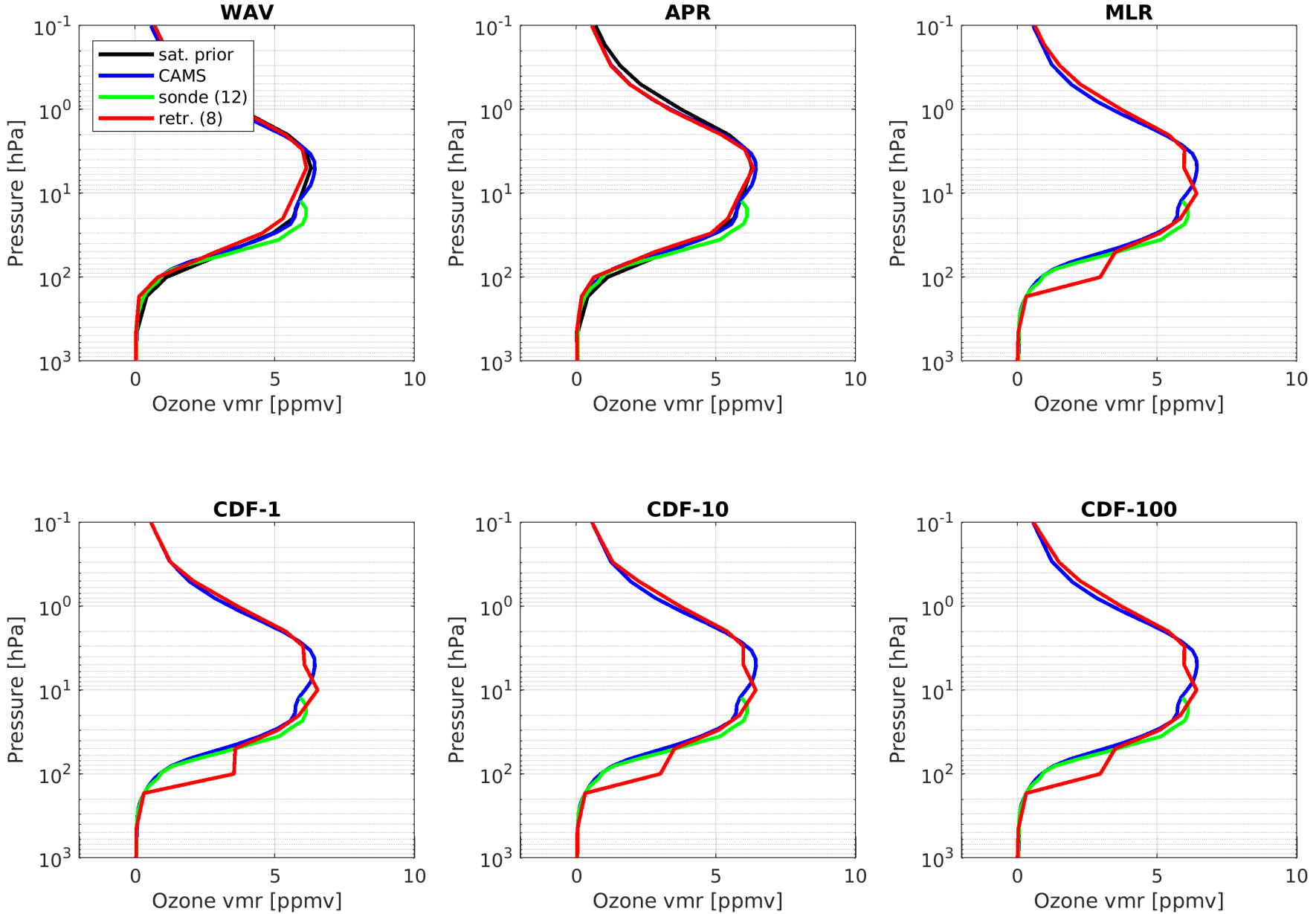


Illustration: RAL OMI v2.14



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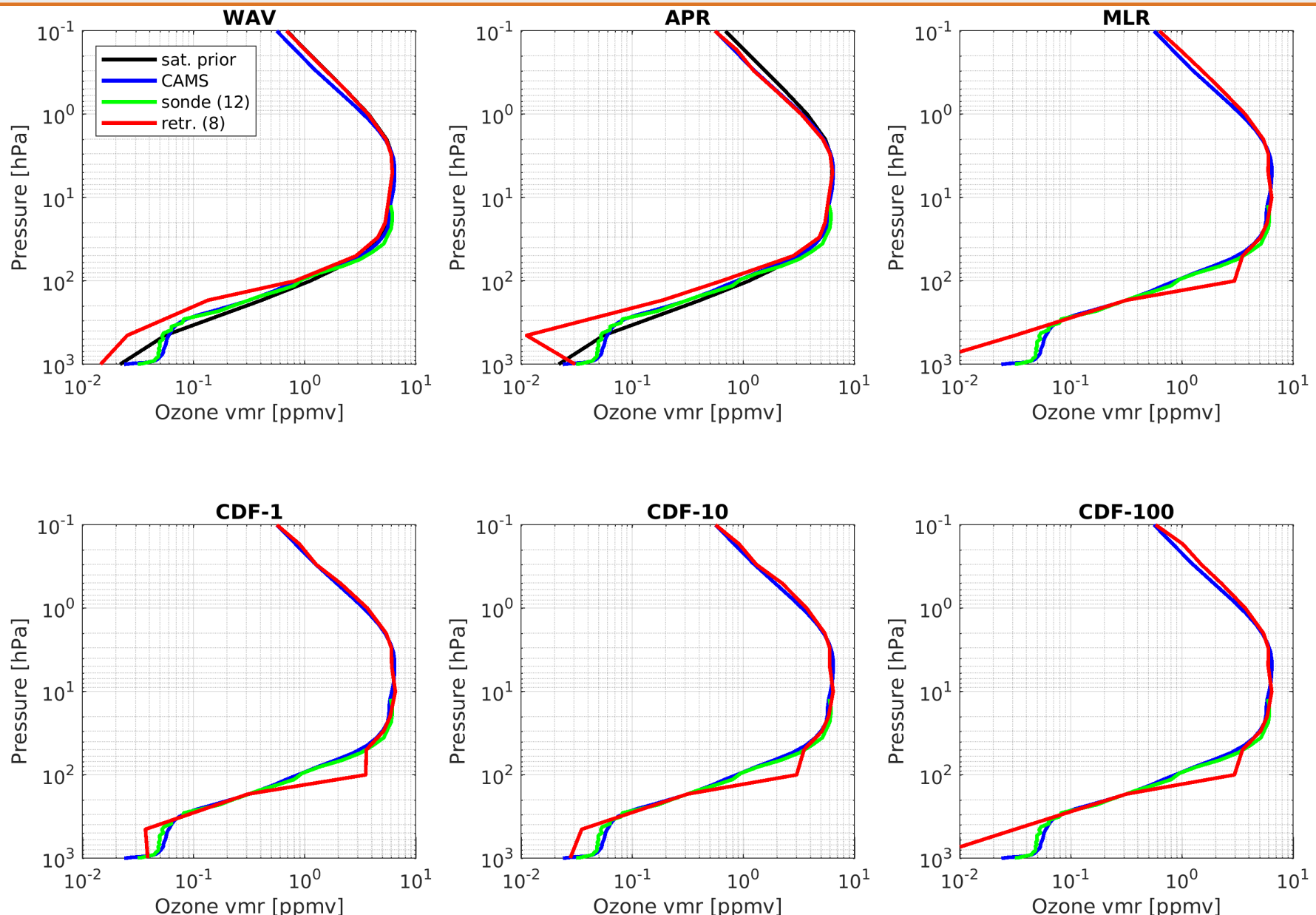
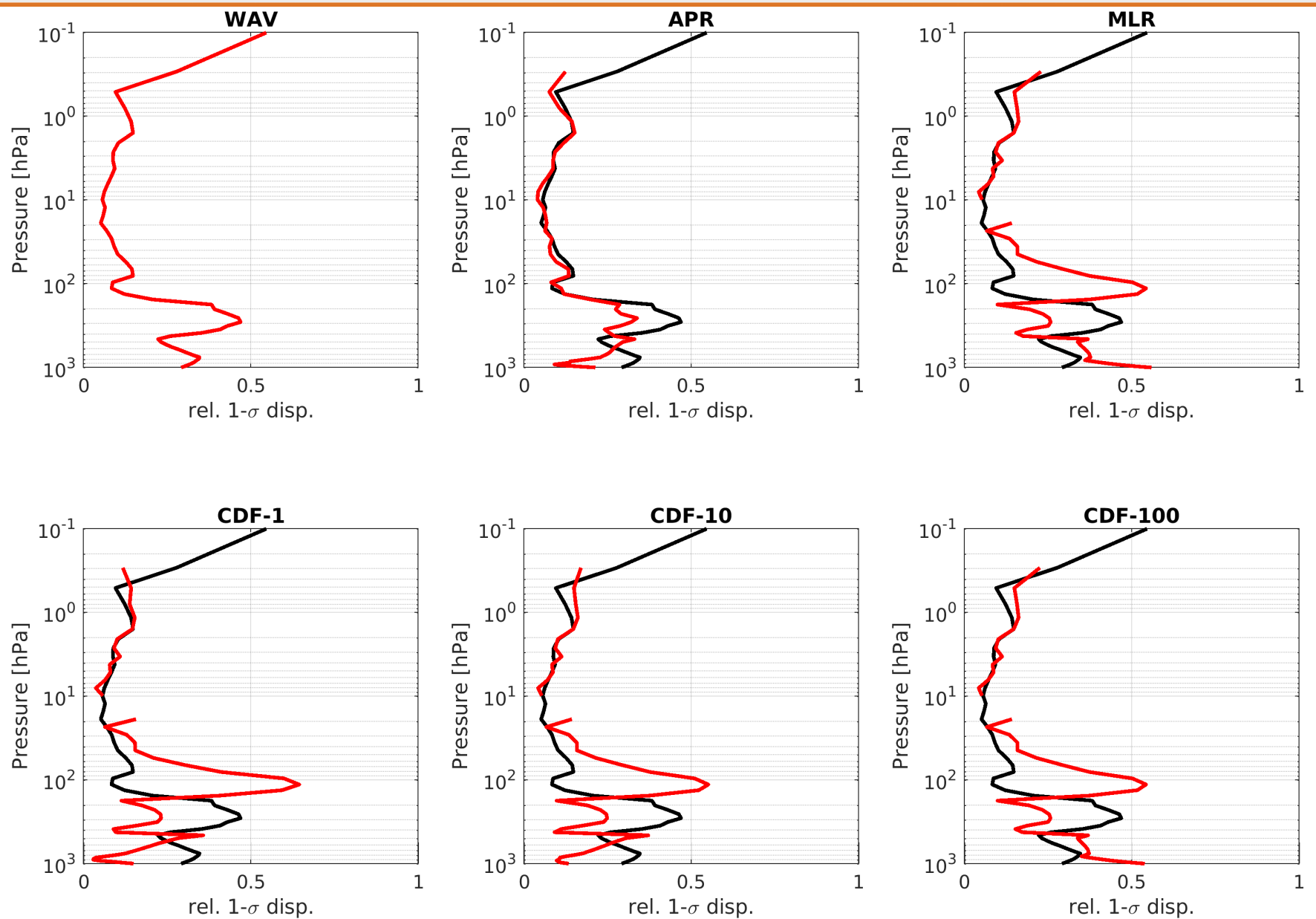


Dispersion reduction upon harmonization? (9 sats)



CEOS VC-20-01: harmonization progress

- (TOAR) tropospheric ozone assessment needs identified
- CAMSRA transfer standard selection / manipulation
- Satellite tropospheric ozone harmonization:
  - Ozone tropospheric columns from vertical correction
  - Ozone profiles from Complete Data Fusion framework: APR, MLR, and CDF (APR method // TOAR-II SOWG approach)
- Next:
  - Harmonization refinements / sensitivity studies / screening
  - Full harmonized time series processing
  - Ground-based quantification of residual discrepancies
- Eventually:
  - Calculating ozone burden (filling of gaps?)
  - Tropospheric ozone assessment studies