TUNER meeting
April 18-20, 2023
KIT

Uncertainty of combined vertically resolved atmospheric state observations from satellites

A. Keppens, D. Hubert, S. Compernolle, and J.-C. Lambert

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TOWARDS UNIFIED ERROR REPORTING

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Previously in your TUNER slideshow…

AMT special issue: “Towards Unified Error Reporting (TUNER)”

Editor(s): T. von Clarmann, D. Degenstein, N. Livesey, and H. Worden

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

Arno Keppens, Steven Compernolle, Tijl Verhoelst, Daan Hubert, and Jean-Christopher Lambert

Atmos. Meas. Tech. 12, 4379–4391, https://doi.org/10.5194/amt-12-4379-2019, 2019

MDPI-RS special issue: “Multi Sensor Data Integration for Atmospheric Composition Analysis”

Editor(s): U. Cortesi and A. Keppens

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

Arno Keppens, Steven Compernolle, Daan Hubert, Tijl Verhoelst, José Granville, and Jean-Christopher Lambert

Remote Sensing 14(9), 2197, https://doi.org/10.3390/rs14092197, 2022

(1) 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)	$\mathbf{S}'(\mathbf{S}^{-1}\boldsymbol{x} - \mathbf{R}_a\boldsymbol{x}_a + \mathbf{R}'_a\boldsymbol{x}'_a)$	$(\mathbf{S}^{-1} - \mathbf{R}_a + \mathbf{R}'_a)^{-1}$	$\mathbf{A} + \mathbf{S}\mathbf{S}_a^{-1} - \mathbf{S}'\mathbf{S}_a'^{-1}$
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)	$\mathbf{A}_{\mathrm{s}}\boldsymbol{x}_{\mathrm{r}} + (\mathbf{I} - \mathbf{A}_{\mathrm{s}})\boldsymbol{x}_{\mathrm{a,s}}$	$\mathbf{A}_{\mathrm{s}}^{1}\mathbf{S}_{\mathrm{r}}(\mathbf{A}_{\mathrm{s}}^{1})^T$	$\mathbf{A}_{\mathrm{s}}$
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	$\boldsymbol{x} - \boldsymbol{\Delta m}$	$\mathbf{S} + \mathbf{S}_{\Delta m}$	$\mathbf{A} - \mathbf{S}_{\Delta m}\mathbf{S}_a^{-1}$

CDF

(von Clarmann and Grabowski, 2007; Keppens et al., 2022)

(2) Deconvolution, for a single profile retrieval

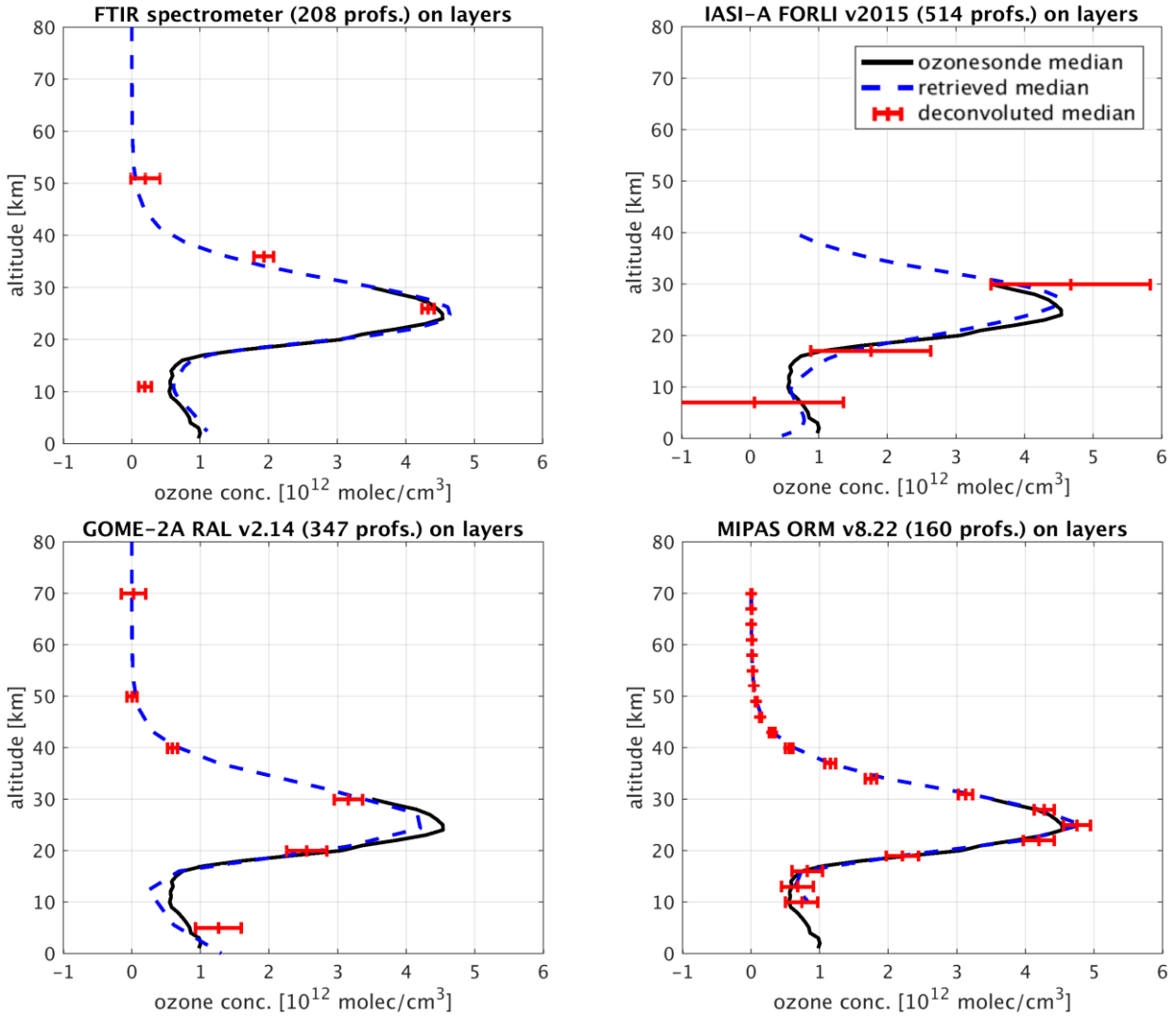
Optimal regridding matrix iteratively:

$$W_{i+1} = \left(W_i^{*T} A^T S^{-1} A W_i^*\right)^{-1} W_i^{*T} A^T S^{-1} A$$

with W_0 an equidistant regridding of choice from x to DOF(x), then

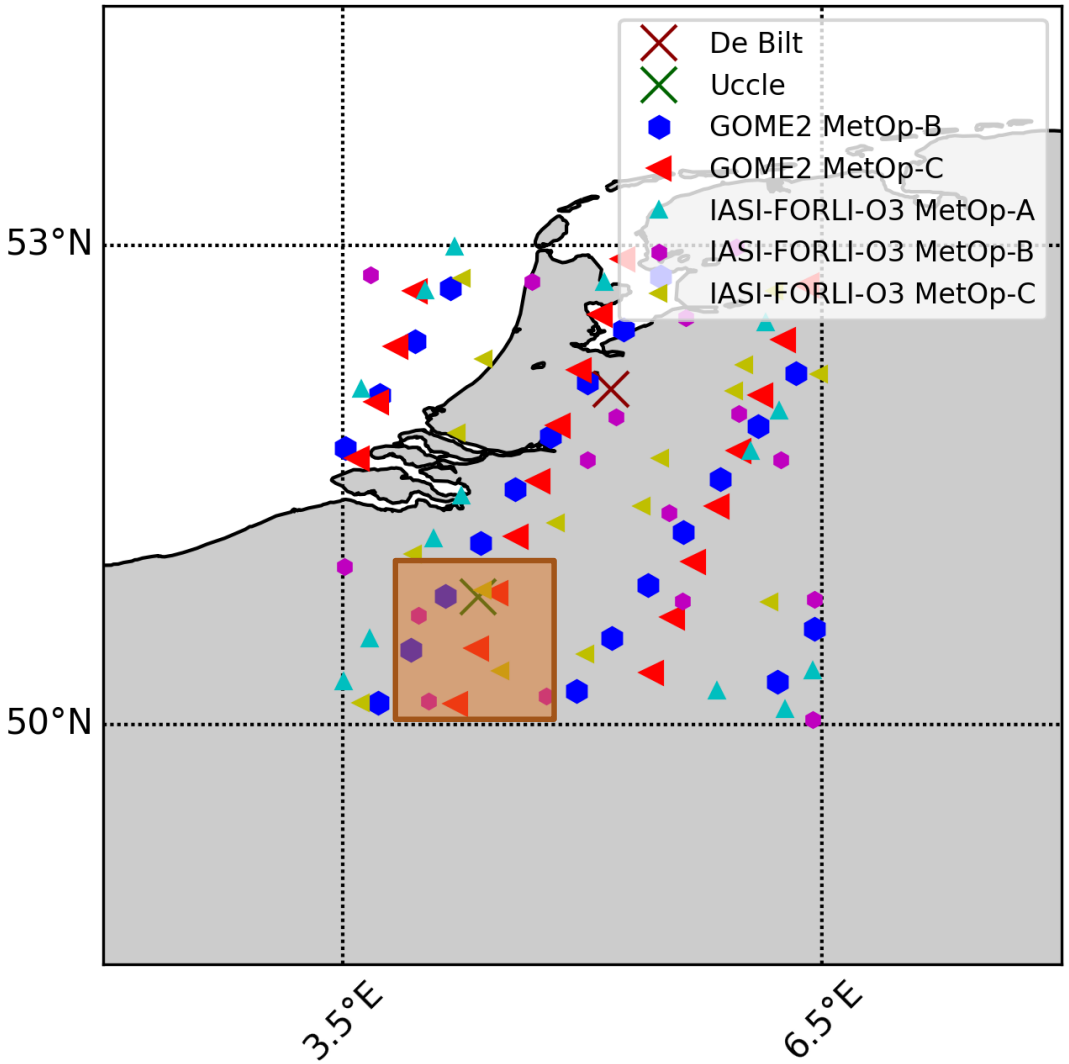
$$x_{ICR} = P[x - (I - A)x_a]$$

with $P = (W_c^{*T} A^T S^{-1} A W_c^*)^{-1} W_c^{*T} A^T S^{-1}$



Build on this for harmonization of TOAR-II data sets

- CEOS Activity VC-20-01, aiming at harmonizing and validating satellite datasets in support of TOAR-II
- Towards monthly-gridded (1°x1°) & harmonized (prior info) satellite L3 data
- Remove prior? But ICR not suitable for tropospheric ozone
- Look into single-sensor vs multi-sensor data fusion
- Example: MetOp overpasses for Brussels on March 24, 2021 – image courtesy of N. Zoppetti (IFAC)



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}	$\left(\sum S_i^{-1} A_i + \alpha S_m^{-1}\right)^{-1} \left(\sum S_i^{-1} [x_i - (I - A_i) x_{a,i}] + \alpha S_m^{-1} x_m\right)$	
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	$I' = W_i W_i^*$ $(\forall i)$	$\left(\sum W_i^{*T} S_i^{-1} A_i W_i^*\right)^{-1}$

CAMS Reanalysis used as a transfer standard

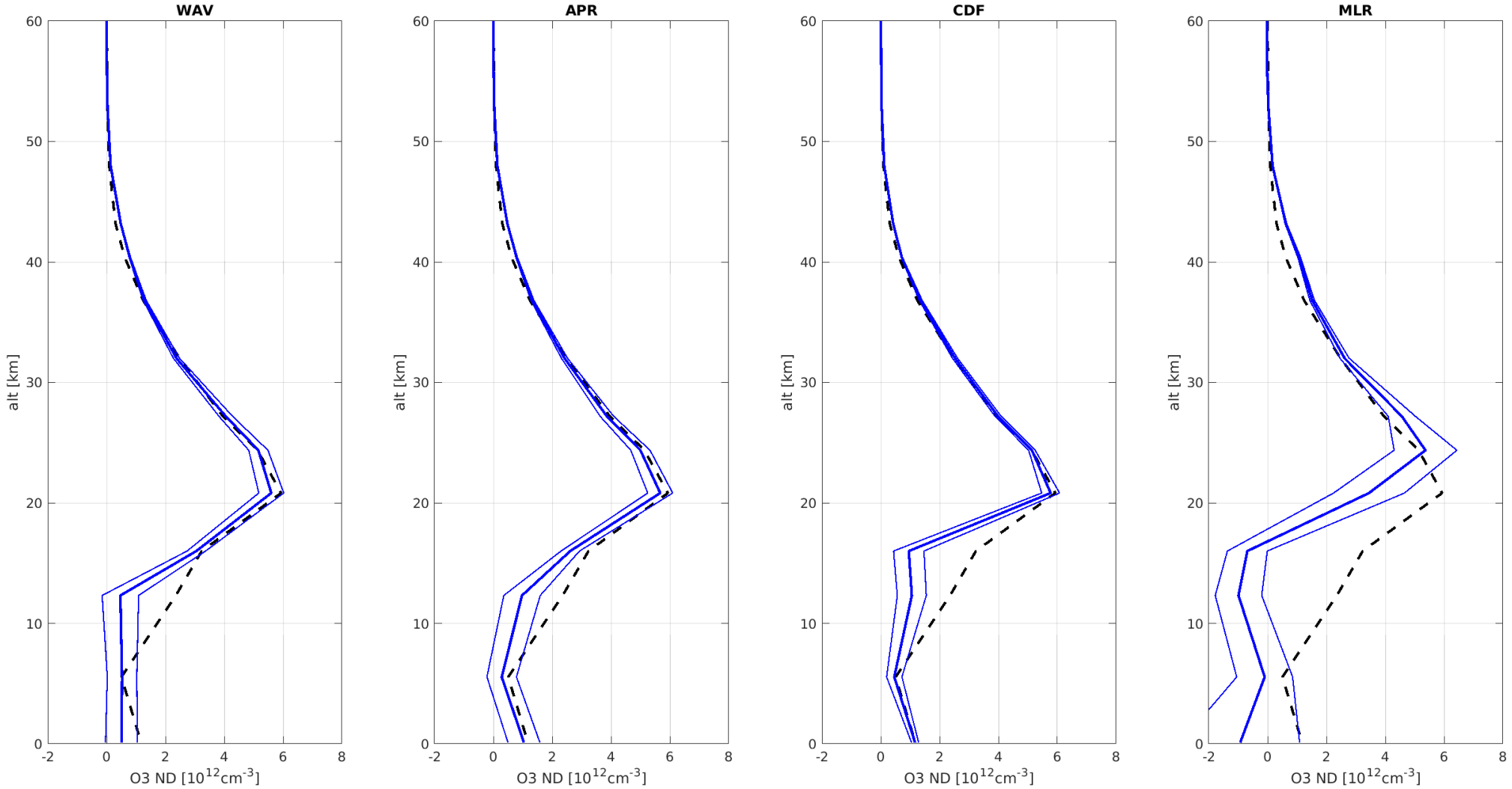
- assimilated ozone: TC (SCIA, OMI, GOME-2A/B), PROF (MIPAS, Aura-MLS, SBUV/2)
- 60 levels (1012-0.1 hPa), 37 levels in troposphere (1012-80 hPa)
- 0.7° x 0.7° (global)
- 6 hourly UTC, but converted to LST noon (2003-2020)

Used for

- vertical correction of tropospheric column (level-3)
- new prior information (including vertical smoothing)
- auxiliary data source for quantity matching
- (assessment of horizontal and temporal sampling differences)

Demonstration: GOME-2B RAL v3

January-March 2020, 1°x1° grid box around Brussels



Prospects

- Understand some of the discrepancies between tropospheric ozone data records from satellites (CEOS VC-20-01 Activity)

- Contribution to TOAR-II Satellite WG and to TOAR-II Special Issue :
  “Harmonization of tropospheric ozone data records from multiple satellites”

- Examine data fusion versus joint retrieval, e.g., for IASI and GOME-2B