Synergetic use of IASI and TROPOMI for generating a tropospheric methane profile product

Matthias Schneider[1], Benjamin Ertl[1,2], Christopher Diekmann[1], Farahnaz Khosrawi[1], Amelie N. Röhling[1], Frank Hase[1] , Darko Dubravica[1], Omaira E. García[3], Eliezer Sepúlveda[3], Alba Lorente[4], Jochen Landgraf[4], Tobias Borsdorff[4], Huilin Chen[5], Rigel Kivi[6], Thomas Laemmel[7], Michel Ramonet[7], Cyril Crevoisier[8], Jerome Pernin[8], Martin Steinbacher[9], Frank Meinhardt[10], Voltaire A. Velazco[11], Nicholas M. Deutscher[12], David Griffith[12], Dave Pollard[13], Hartmut Bösch[14], Tim Trent[14], Harald Sodemann[15]

[1]Institute of Meteorology and Climate Research (IMK-ASF), Karlsruhe Institute of Technology, Karlsruhe, Germany
[2]Steinbuch Centre for Computing (SCC), Karlsruhe Institute of Technology, Karlsruhe, Germany
[3]Izana Atmospheric Research Center, Agencia Estatal de Meteorología (AEMET), Santa Cruz de Tenerife, Spain
[4]Earth Science Group, SRON Netherlands Institute for Space Research, Utrecht, The Netherlands
[5]Center for Isotope Research, University of Groningen, Groningen, The Netherlands
[6]Space and Earth Observation Centre, Finnish Meteorological Institute, Sodankylä, Finland
[7]Laboratoire des Sciences du Climat et de l'Environnement (LSCE), CEA, 91191 Gif sur Yvette, France
[8]Laboratoire de Météorologie Dynamique (LMD), Palaiseau, France
[9]Swiss Federal Laboratories for Materials Science and Technology (EMPA), Dübendorf, Switzerland
[10]Air Monitoring Network, Federal Environment Agency (UBA), Langen, Germany
[11]Deutscher Wetterdienst, Albin-Schwaiger-Weg 10, Hohenpeissenberg, Germany
[12]Centre for Atmospheric Chemistry, School of Earth, Atmospheric and Life Sciences, Faculty of Science, Medicine and Health, University of Wollongong, Wollongong, Australia
[13]National Institute of Water and Atmospheric Research Ltd (NIWA), Lauder, New Zealand
[14]EOS Research Group, University of Leicester University Road, Leicester, LE1 7RH, UK
[15]Geophysical Institute and Bjerknes Centre for Climate Research, Bergen, Norway

1: MUSICA IASI products
2: Combination of IASI and TROPOMI products
- Method
- Example 1: methane
- Example 2: water vapour isotopologues

3: Summary and outlook

See also: https://doi.org/10.5194/amt-2021-31

https://doi.org/10.5194/amt-2021-31
Preprint. Discussion started: 23 February 2021

Atmospheric Measurement Techniques Discussions
Open Access
EGU

Synergetic use of IASI and TROPOMI space borne sensors for generating a tropospheric methane profile product

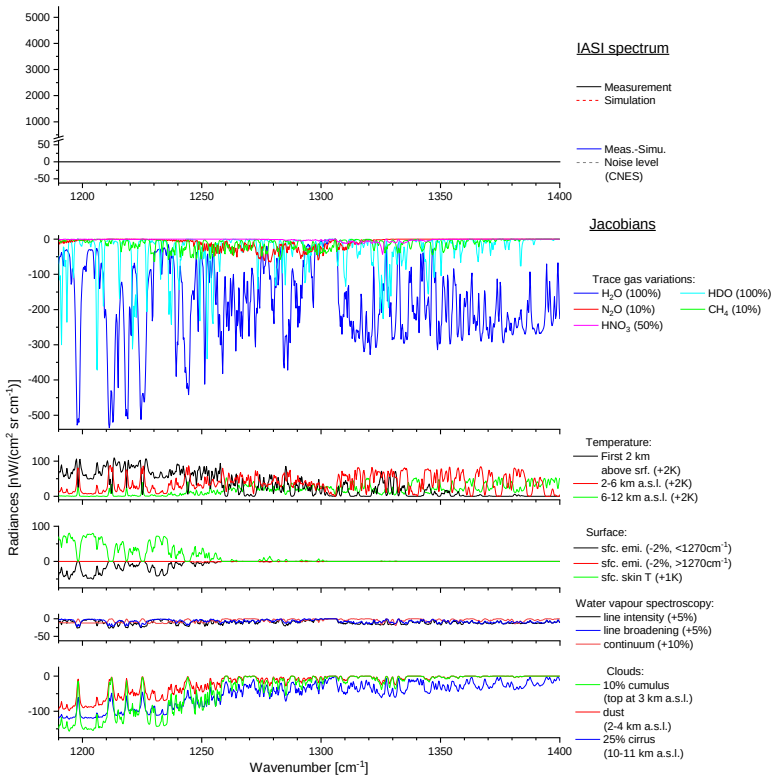
Matthias Schneider[1], Benjamin Ertl[1,2], Christopher J. Diekmann[1], Farahnaz Khosrawi[1], Amelie N. Röhling[1], Frank Hase[1], Darko Dubravica[1], Omaira E. García[3], Eliezer Sepúlveda[3], Tobias Borsdorff[4], Jochen Landgraf[4], Alba Lorente[4], Huilin Chen[5], Rigel Kivi[6], Thomas Laemmel[7,*], Michel Ramonet[7], Cyril Crevoisier[8], Jérome Pernin[8], Martin Steinbacher[9], Frank Meinhardt[10], Nicholas M. Deutscher[11], David W. T. Griffith[11], Voltaire A. Velazco[11,**], and David F. Pollard[12]

MUSICA IASI products

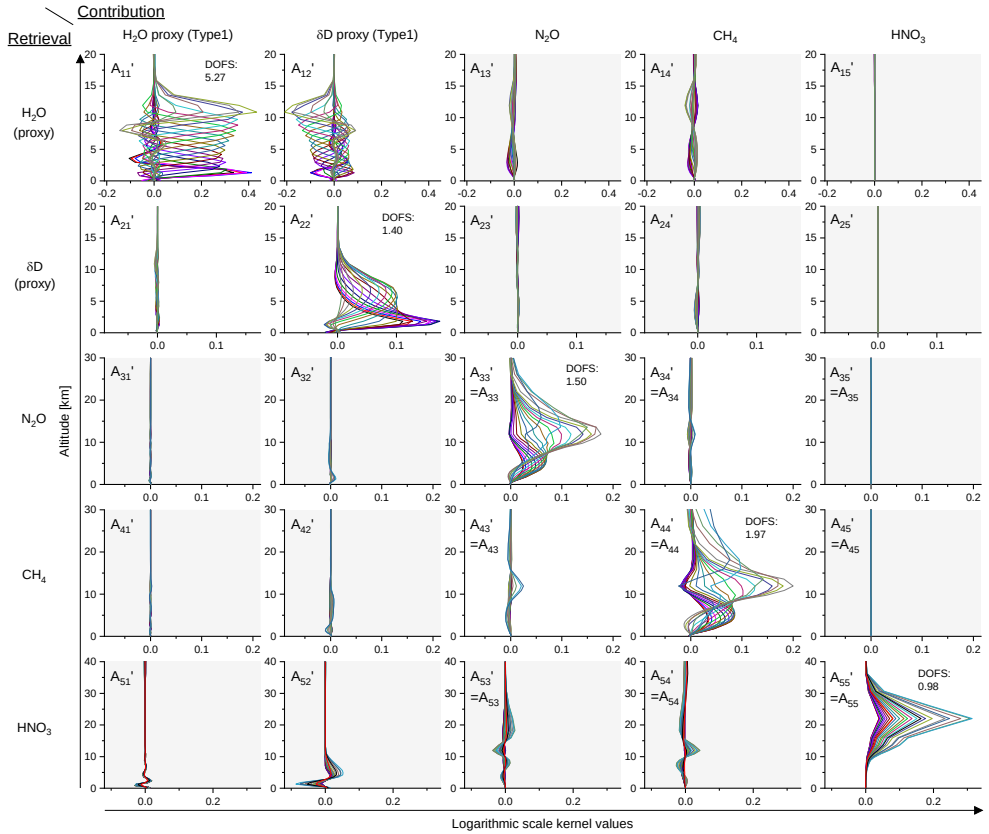
MUSICA IASI (A + B (+C), retrieval setup

Code: PROFFIT-nadir; different retrieval products: H_2O, δD, N_2O, CH_4, and HNO_3

Spectra and Jacobians



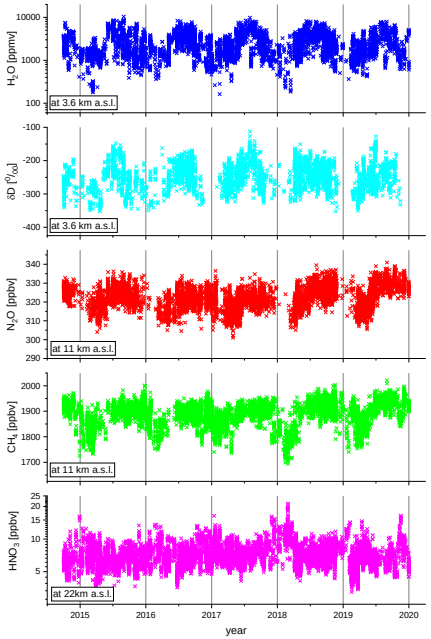
Full state averaging kernels



MUSICA IASI products

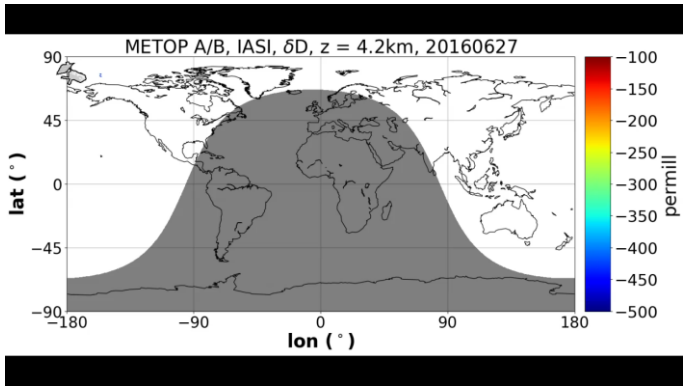
MUSICA IASI (A + B (+C), global, 2014-2020, ≈ 1.5bn retrievals)

Time series over Karlsruhe



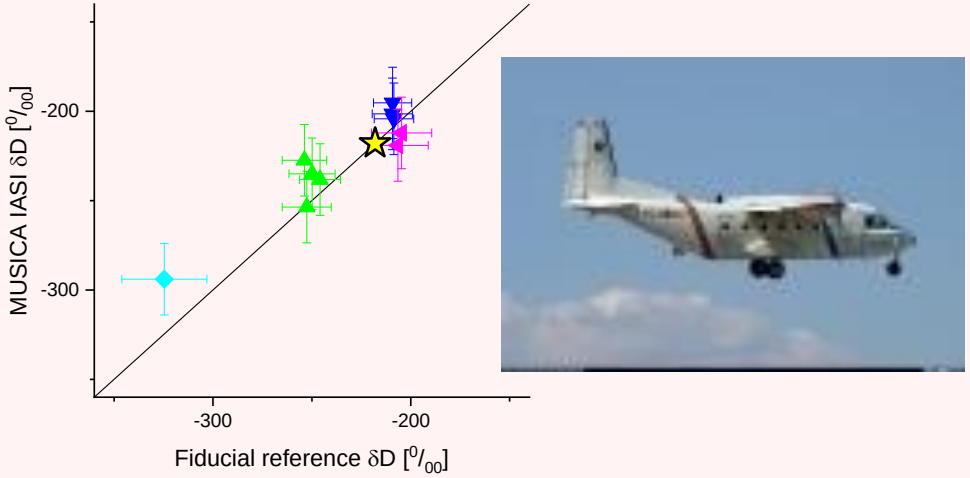
Many validation studies:
Schneider et al. (2016), Borger et al. (2018), García et al. (2018), etc.

Overpasses 20160627



≈300000 morning observations per day (local time 9:30)
≈ 300000 evening observations per day (local time 21:30)

Example of MUSICA IASI fiducial referencing: δD



Method: updating a MUSICA IASI profile product with information from a TROPOMI total column product

Data assimilation formalism:

$$x^a = x^b + \mathbf{G}[y - \mathbf{H}x^b]$$
$$\mathbf{G} = \mathbf{S}^b\mathbf{H}^T[\mathbf{H}\mathbf{S}^b\mathbf{H}^T + \mathbf{S}_\varepsilon]^{-1}$$

Input

x^b: background state vector

→ **MUSICA IASI profile product**

$\mathbf{S}^b$: background state error covariances

→ **MUSICA IASI a posteriori covariances**

y: measurement state vector

→ **TROPOMI total column product**

$\mathbf{H}$: measurement forward operator

→ **TROPOMI total column kernel**

$\mathbf{S}_\varepsilon$: measurement state error covariances

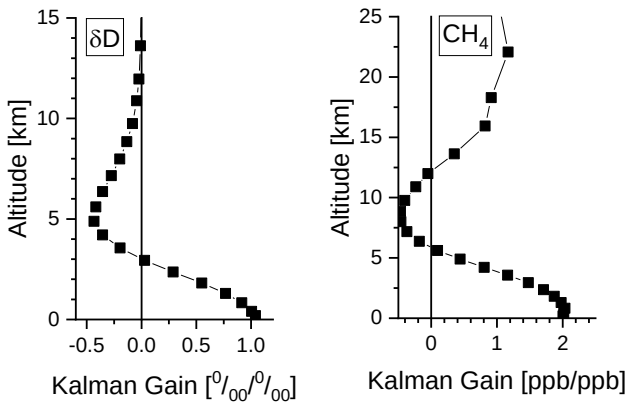
→ **TROPOMI total column noise**

Output:

x^a: analysed state vector

$\mathbf{G}$: Kalman gain matrix

Kalman Gain

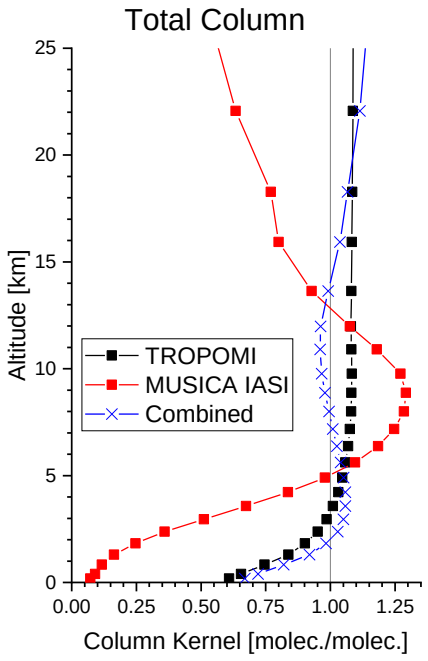


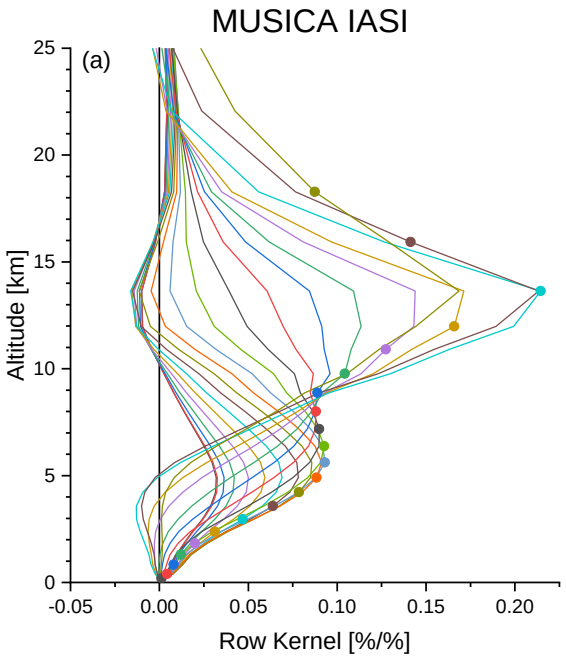
Differences between the IASI and TROPOMI total columns will have the strongest impact in the lower troposphere.

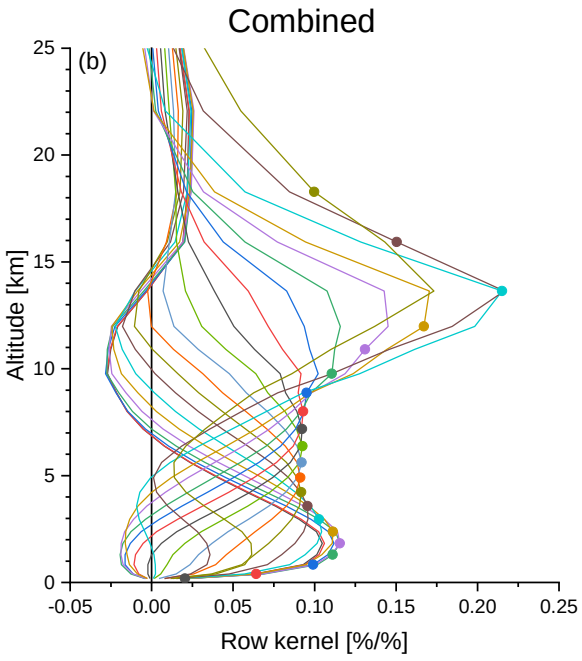
For linear and "moderately non-linear" problems and adjusted IASI and TROPOMI a priori information, this analysed state vector (x^a) is identical to an optimal estimation retrieval that uses a combined {IASI,TROPOMI} measurement state vector.

Example 1: methane (CH_4), effect of combination on the averaging kernels

We use the TROPOMI XCH4 product
as described in Lorente et al. (2021)

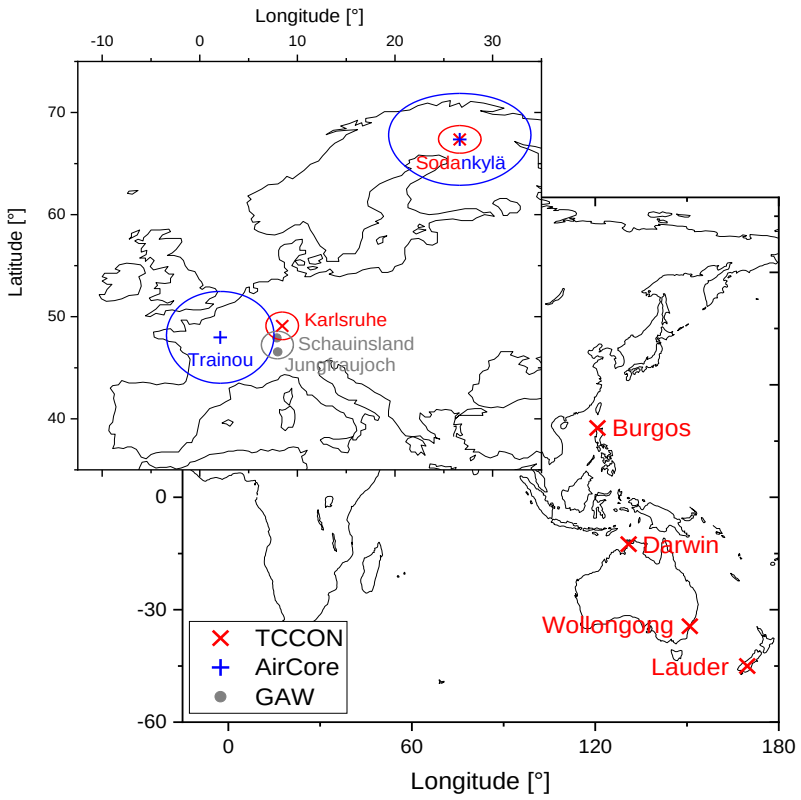




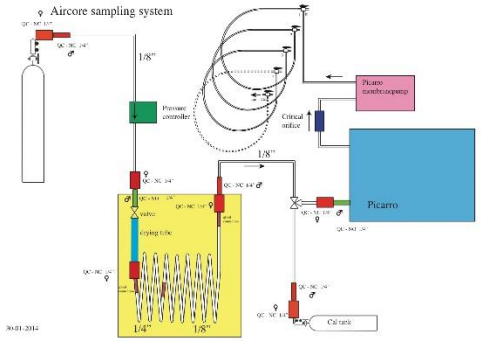


Example 1: CH_4 validation references

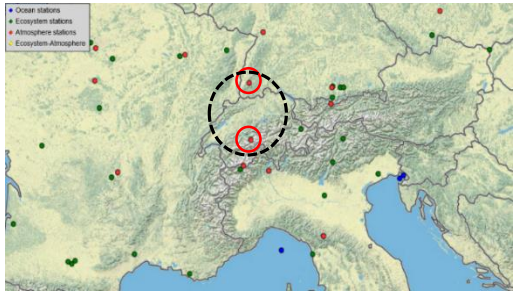
TCCON: for XCH_4
AirCore: for CH_4 in the UTLS
GAW: for CH_4 in the troposphere

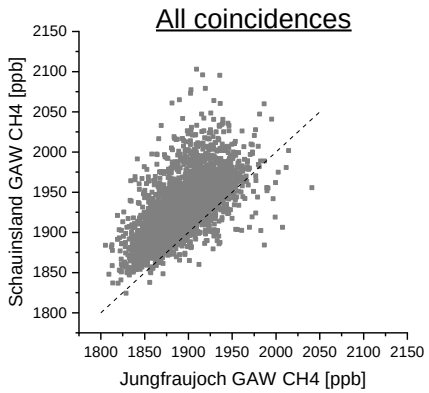


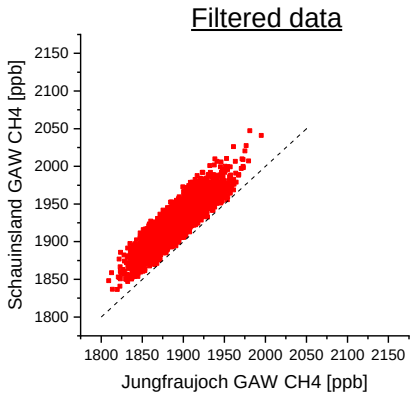
AirCore: balloon-based in-situ sampling



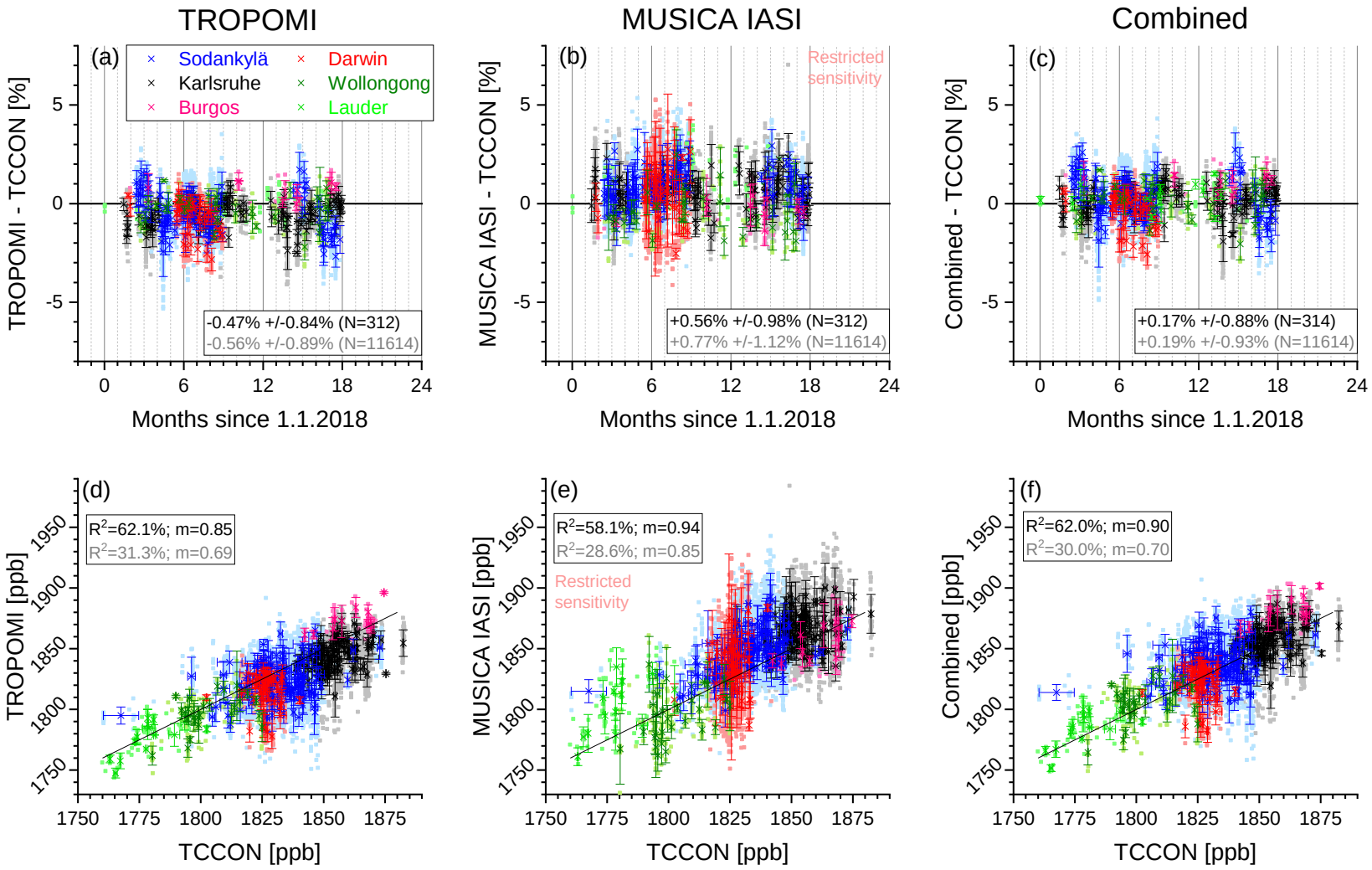
Common signals in two nearby GAW stations are well representative for tropospheric CH_4





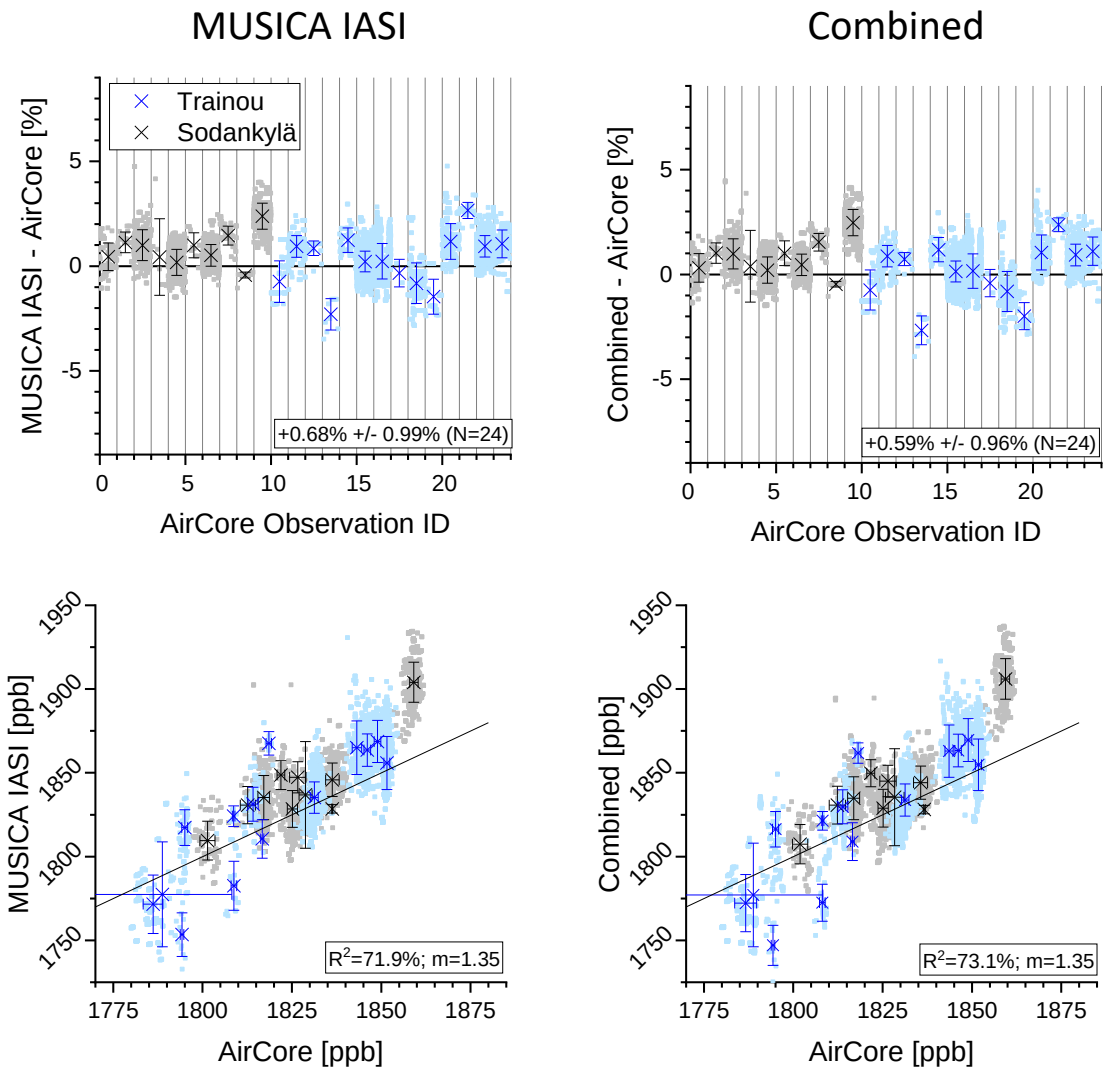


Example 1: validation of XCH_4



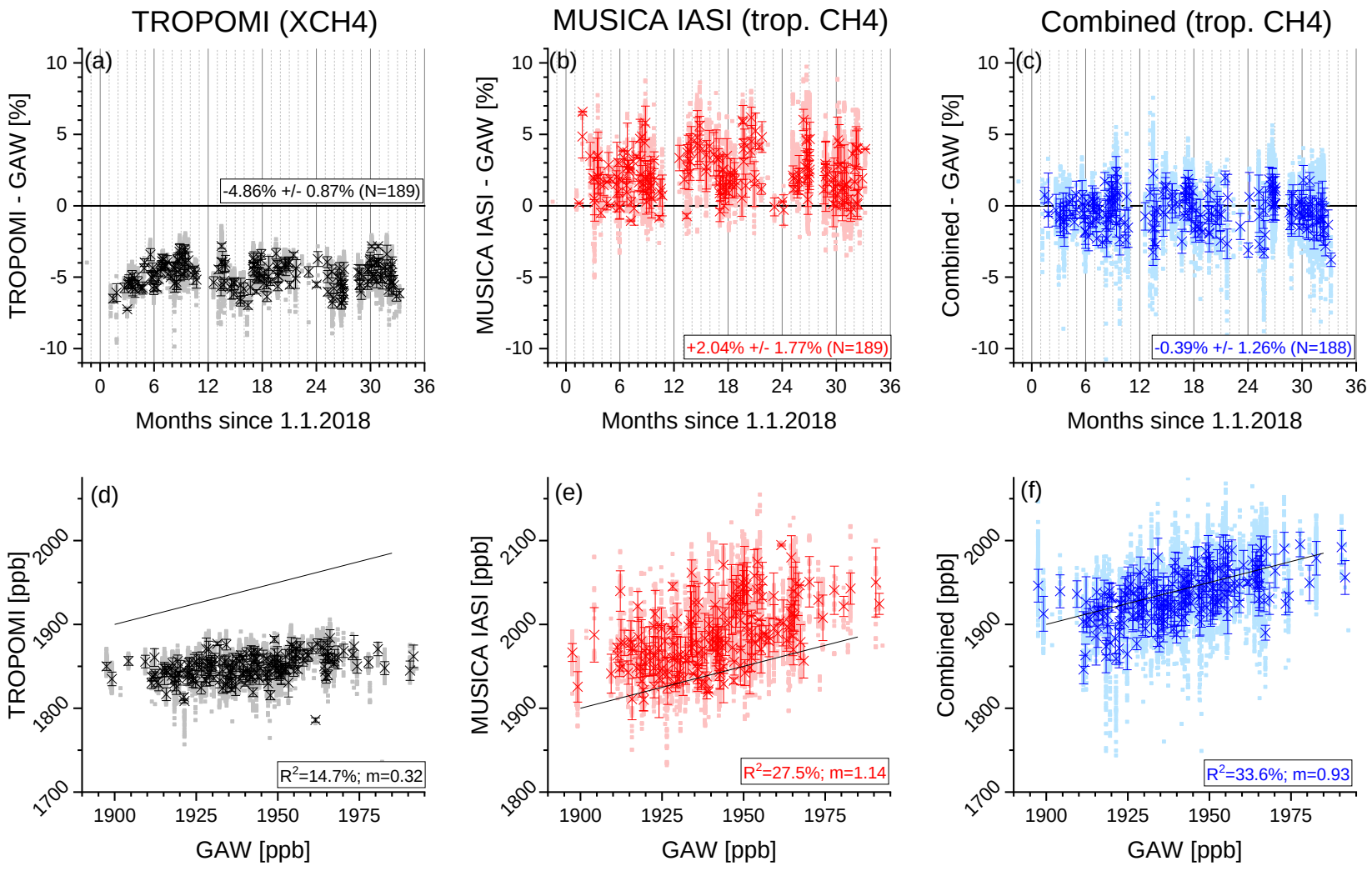
Combined as good as TROPOMI

Example 1: validation of CH_4 in the UTLS



Combined as good as MUSICA IASI

Example 1: validation of CH_4 in the troposphere



Combined much better than TROPOMI or MUSICA IASI: synergetic benefit for tropospheric CH_4!

Example 2: water vapour isotopologue ratios (δD)

The interesting quantity is the **ratio** between H2O and HDO, expressed as δD

<u>Problem:</u> we need an analytic framework for ratio remote sensing data

<u>Solution (developed during MUSICA):</u>

(1) transfer the problem to the logarithmic scale: $\partial \ln x = \frac{1}{x}\partial x$

(2) use proxy state: $\ln\left[\frac{\hat{x}_{\mathrm{HDO}}}{\hat{x}_{\mathrm{H2O}}}\right] = \ln \hat{x}_{\mathrm{HDO}} - \ln \hat{x}_{\mathrm{H2O}}$

<u>Transformation</u>:

{H_2O,HDO} state

→

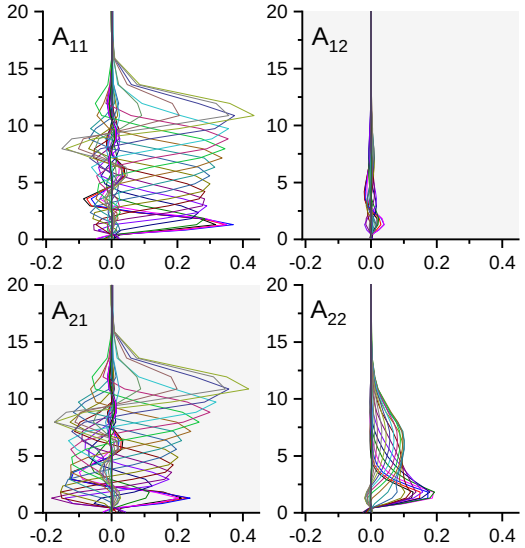
{H_2O,δD} proxy-state

$$\mathrm{A_p} = \mathrm{P}\,\mathrm{A_{log}}\,\mathrm{P}^{-1}.$$

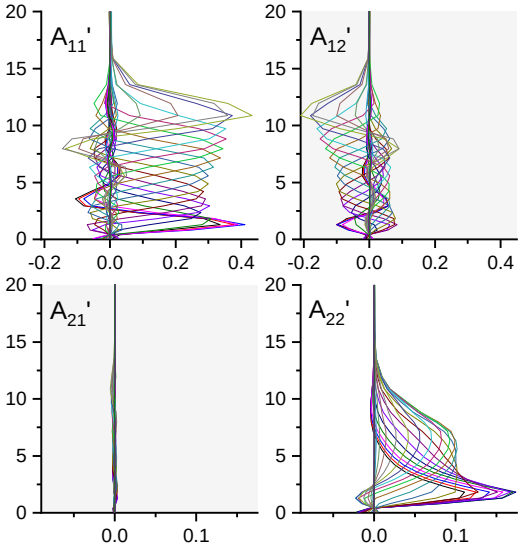
Transformation matrix P for {H_2O,δD} proxy-state :

$$\mathrm{P} = \begin{pmatrix} +0.5 & \cdots & 0 & +0.5 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & +0.5 & 0 & \cdots & +0.5 \\ -1.0 & \cdots & 0 & +1.0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & -1.0 & 0 & \cdots & +1.0 \end{pmatrix}$$

Kernel: $\mathbf{A}$



Proxy kernel: $\mathbf{A_p}$



… analytic framework for **ratio** remote sensing data

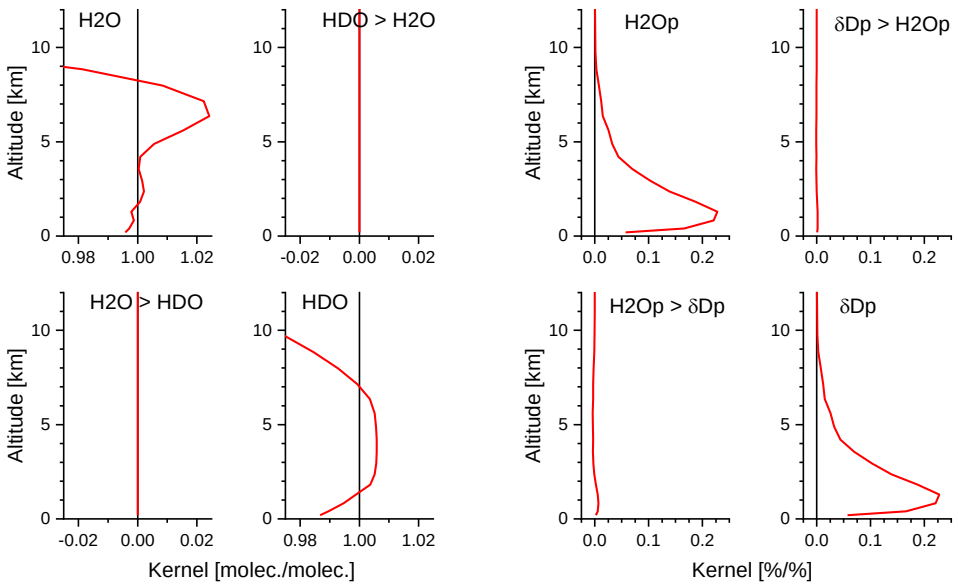
Extension to column products:

$a_p^T = \mathrm{P_X}\,\mathrm{M_X^{-1}}\,\mathrm{H_X^{-1}}\,a^T\mathrm{H}\,\mathrm{M}\,\mathrm{P}^{-1}$,

with

$$\mathrm{H} = \begin{pmatrix} h_1 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & h_N & 0 & \cdots & 0 \\ 0 & \cdots & 0 & h_1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & 0 & \cdots & h_N \end{pmatrix}; \quad \mathrm{H_X} = \begin{pmatrix} \sum_{i=1}^{i=N} h_i & 0 \\ 0 & \sum_{i=1}^{i=N} h_i \end{pmatrix}; \quad \mathrm{M_X} = \begin{pmatrix} \hat{X}_{\mathrm{H2O}} & 0 \\ 0 & \hat{X}_{\mathrm{HDO}} \end{pmatrix}; \quad \mathrm{P_X} = \begin{pmatrix} +0.5 & +0.5 \\ -1.0 & +1.0 \end{pmatrix}.$$

Column kernel: a^T Proxy column kernel: a_p^T

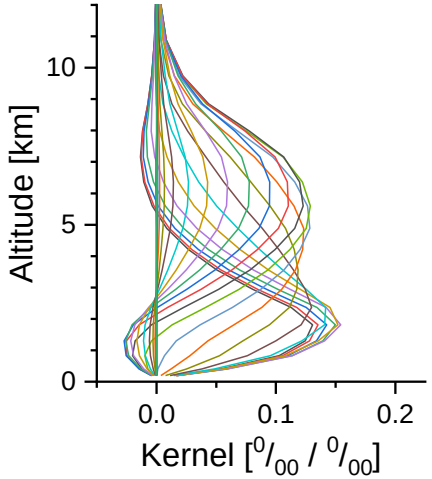


Example 2: Combination, effect on the averaging kernels

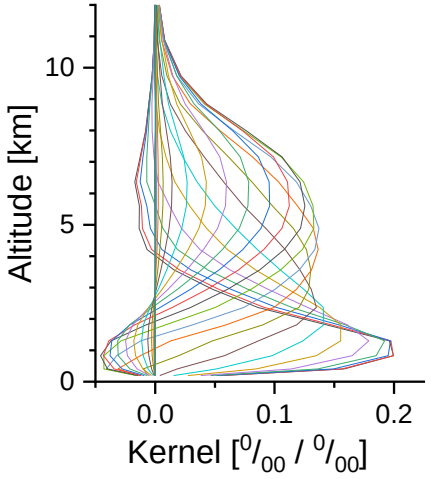
Here we use the XδD TROPOMI product of UoL-FP v0.9.4.

Proxy averaging kernels

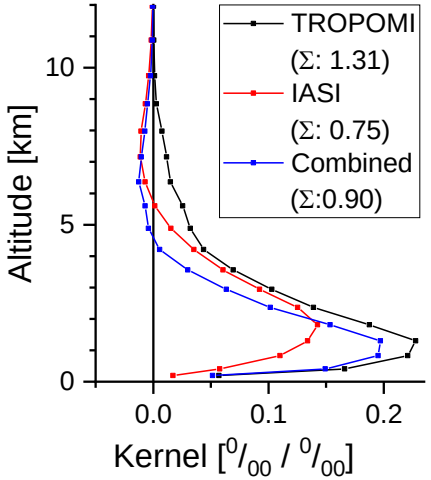
MUSICA IASI retrieval



MUSICA IASI retrieval with TROPOMI "assimilated"



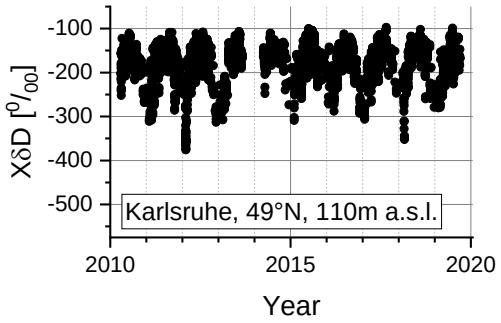
Comparison, column kernels



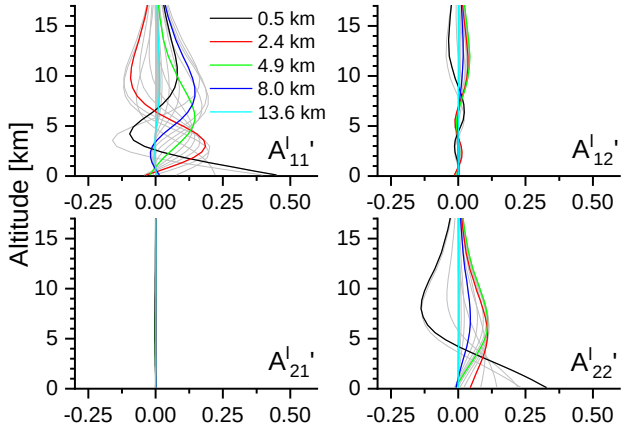
Example 2: Validation of surface-near data product

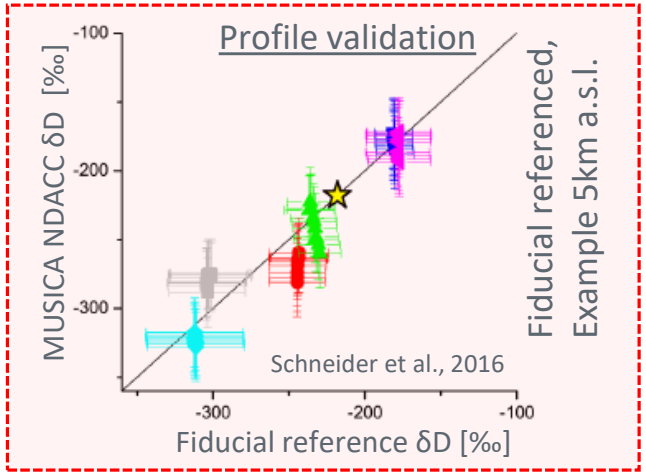
Validation reference: MUSICA NDACC profile data at Karlruhe (49°N)

Temporal coverage



Proxy kernel

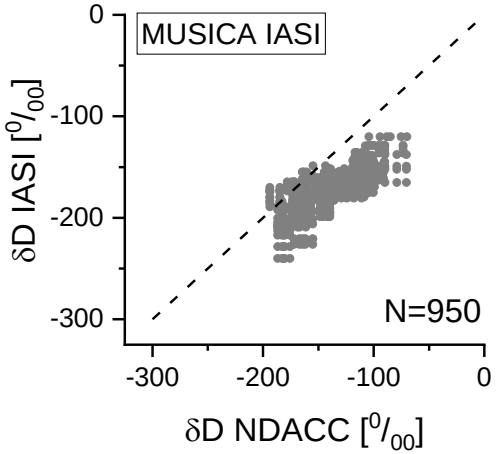


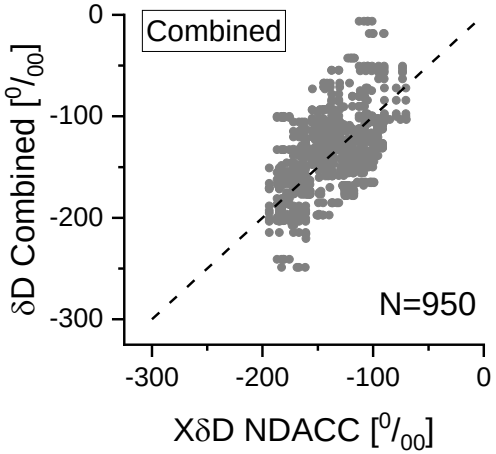


Validation for individual observations, surface-near data product

Validation for 900m a.s.l.

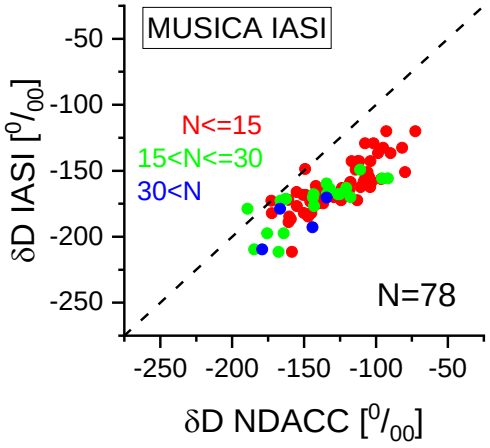
Collocations:
(1) within 4h
(2) within 50km

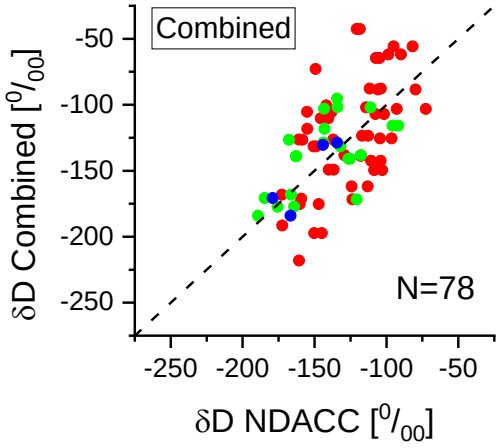




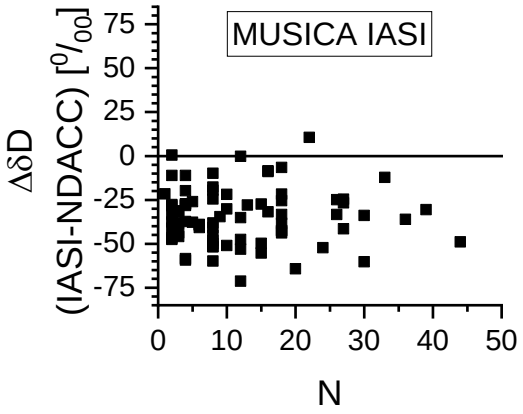
Example 2: Validation, surface-near data product

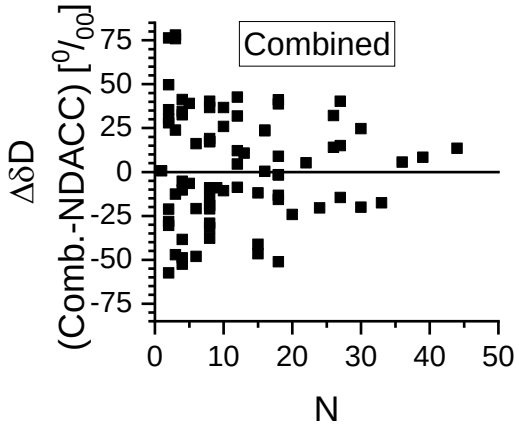
Comparisons of 4-hourly means





Impact of averaging:





For combined data: when averaging 20 data points, scatter is within 25‰.

Summary and Outlook

- The MUSICA IASI data set is of very good quality and very comprehensive. It contains all info needed for its combination with other products: a priori, AVKs, and error covariances.
- Combination with TROPOMI XCH_4: capability to resolve tropospheric layer from ground to about 6 km above ground independently from the UTLS.
- Validation results: agreement within 1% with references and scatter wrt references of 1-1.5%
- Combination with TROPOMI XδD. Combination of ratio data is particularly complex but first studies look promising: lower tropospheric layer (ground – 2.5 km above ground) can be detected independently from free troposphere (3 – 6 km above ground).
- Outlook: IASI and TROPOMI successors will be together on the Metop Second Generation satellites, perfect for collocation, very promising!

<u>Acknowledgement:</u> TCCON data provided by TCCON partners, AirCore data provided by AirCore partners, CH4 GAW data provided by EMPA and UBA, TROPOMI XδD data (provided by ESA, project S5P+I_H2O-Iso), MUSICA IASI data generated with ForHLR (funded by BW and GER) and during DFG projects MOTIV and TEDDY.