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Institute of Meteorology and Climate Research
Atmospheric Trace Gases and Remote Sensing

The comprehensive multi-annual MUSICA IASI dataset of daily global free tropospheric {H_2O, δD}-pairs: product demonstration

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References:
[1] Schneider, 2016, doi: 0.5194/amt-9-2845-2016
[2] Garcia, 2018, doi: 10.5194/amt-11-4171-2018
[3] https://www.eumetsat.int

Abstract We present the new MUSICA (*Multi-platform remote Sensing of Isotopologues for investigating the Cycle of Atmospheric water*) IASI tropospheric $\{H_2O, \delta D\}$ – pair product. By providing high-resolution spectra on an operational and global basis, the thermal infrared sensor IASI onboard the polar-orbiting Metop satellites has great potential for atmospheric composition studies. Based on Schneider et al. (2016), an optimized processing chain has recently been developed to efficiently retrieve water vapour isotopologues (H_2O and HDO/H_2O) as well as CH_4, N_2O and HNO_3 from the huge amount of freely available IASI spectra [1, 2]. Using the improved MUSICA IASI processing, we created a global and daily dataset of combined $\{H_2O, \delta D\}$ – pairs for the continuous period 2016 – 2018 with best sensitivities at 760 – 540 hPa (≈ 2.5 – 5 km). Moreover, about 30% of the processed retrievals provide vertical profile information, i.e. information on $\{H_2O, \delta D\}$ – pairs for two vertically separated tropospheric layers.

The Metop IASI mission

Sensor type	nadir thermal infrared
Measurements	90.000 spectra per orbit 14 orbits per day and satellite ➢currently two satellites: 2.5 Mio spectra per day
Global coverage	twice per day overpasses at ~9:30 and 21:30 local time
Pixel size at nadir	12 km

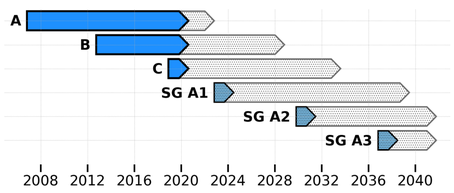

Fig. 1: *Timeline of the current and future Metop satellites carrying the sensor IASI [3].*

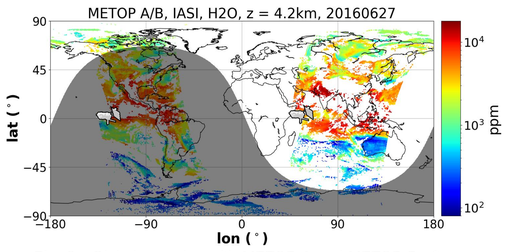

Fig. 2 : *Global scanning with METOP-A and METOP-B after 5.5h of orbiting at 27.06.2016.*

The MUSICA IASI processing

1. a priori selection	cloud-free pixels reliable temperature retrievals from EUMETSAT ➢ spectra amount reduced to ~30%
2. retrieval algorithm	simultaneous optimal estimation retrieval for $H_2O, \delta D, CH_4, N_2O$ and HNO_3
3. a posteriori evaluation	quality screening for good sensitivity with respect to $\{H_2O, \delta D\}$ – pairs ➢ data reduction to ~20% (≈ 0.5 Mio. reliable $\{H_2O, \delta D\}$ – pair observations per day)

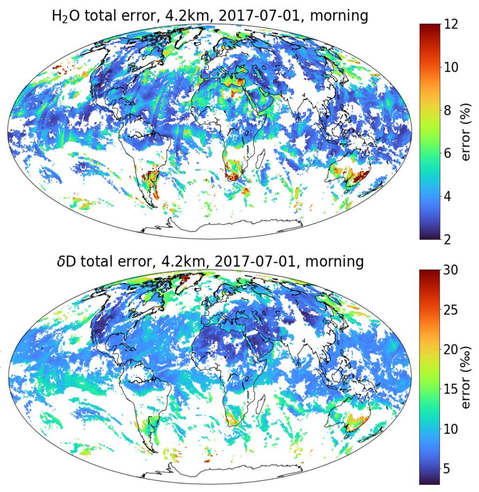

Fig. 3: *Total errors for the retrieved H_2O (top) and δD (bottom) for 01.07.2017. Temperature uncertainties and measurement noise are the leading errors.*

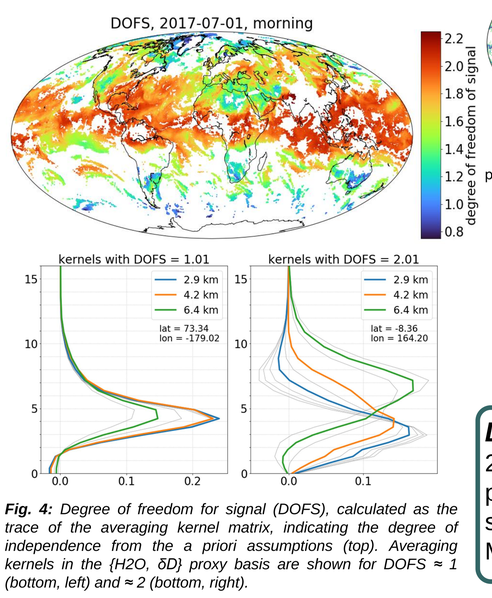

Fig. 4: *Degree of freedom for signal (DOFS), calculated as the trace of the averaging kernel matrix, indicating the degree of independence from the a priori assumptions (top). Averaging kernels in the {H2O, δD} proxy basis are shown for DOFS ≈ 1 (bottom, left) and ≈ 2 (bottom, right).*

Geographical representativeness

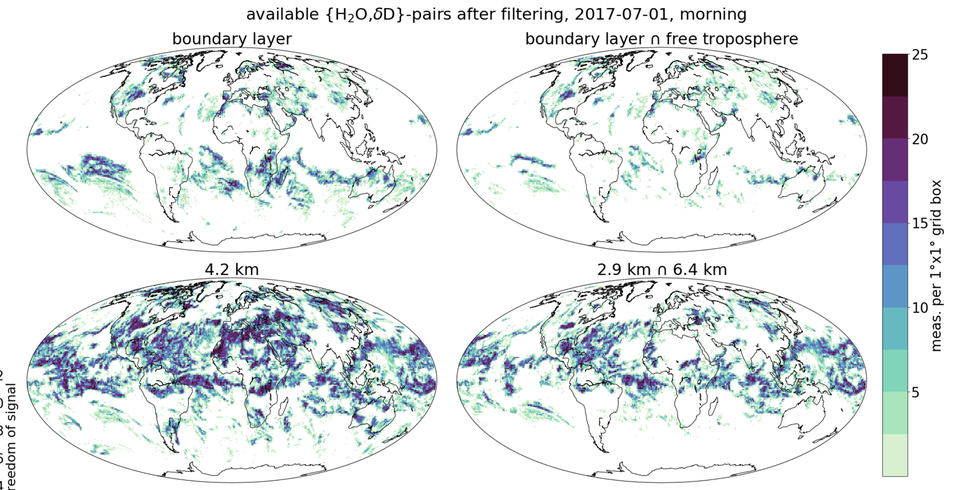

Fig. 5 (above): *Amount of a posteriori evaluated {H_2O,δD} - pairs per 1°x1° grid box for 01.07.2017, for different height levels (top row: terrain-following layers, bottom row: fixed heights.*
The two right plots indicate the events where isotopologue data are available at both the two given height levels after respective filtering. These events are thus assumed to contain vertical profile information between the two defined levels.

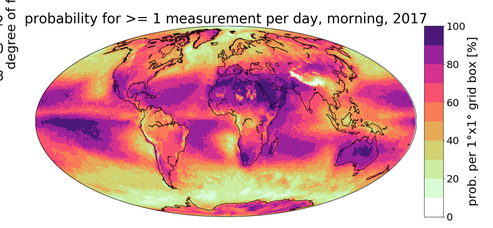

Fig. 6 (left): *Probability of at least one measurement occurring per day and per 1°x1° grid box at 4.2km, after the MUSICA a posteriori evaluation and filtering.*

Data Availability The full MUSICA processing has been performed for Summer 2013 and the continuous period 2016 – 2018. Further processing is currently being performed for 2014 – 2015 and for 2019. In total, ~ 1 000 Mio. individual spectra will soon be processed. For accessing the processed MUSICA IASI data please contact Matthias Schneider (matthias.schneider@kit.edu).

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KIT – The Research University in the Helmholtz Association

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References:
[1] Schneider, 2017, doi: 10.5194/amt-10-507-2017
[2] Eckstein, 2018, doi: 10.5194/gmd-11-5113-2018
[3] Weber, 2019, doi: 10.5281/zenodo.3360021
[4] Campello, 2013, doi: 10.1007/978-3-642-37456-2_14
[5] Ertl, 2019, doi: 10.5281/zenodo.3265957
[6] Pfahl, 2012, doi: 10.5194/acp-12-1629-2012
[7] Yoshimura, 2011, doi: 10.1029/2011JD016035

Abstract We highlight ongoing studies and projects with focus on global tropospheric a posteriori evaluated $\{H_2O, \delta D\}$ – pair data for the continuous period 2016 – 2018. Several international projects involve the investigation and application of MUSICA IASI $\{H_2O, \delta D\}$ – pairs. The scientific objectives are to use global MUSICA IASI data for investigating the links between isotopologues and atmospheric processes in terms of heating, microphysics and dynamics. In addressing these issues, cross-comparisons with isotope-enabled models play a crucial role. Further we perform intercomparison and validation studies with other remote sensing products. Here one of the long-term objectives is to develop techniques for merging satellite products with differing sensitivities.

Comparisons with model data

For reliable comparisons with isotope-enabled models it is highly recommended to consider the limited vertical resolution and sensitivity of the IASI observations.
The relation between a retrieved IASI state ($\hat{x}$) to the real atm. state (x) and the assumed a priori state (x_a) is described by the averaging kernel matrix (A):

$$\hat{x} = A\,(x\, - x_a) + x_a$$

By setting the modeled state as x and determining the averaging kernels A for the atmospheric conditions in the model, this relation can be used to simulate a transformed state $\hat{x}$ that reflects how the IASI sensor would observe the modeled atmosphere. A is calculated based on radiative transfer assumptions [1, 2].

Data storage and compression

Due to the huge data amount it is worth considering techniques aiming at efficient data storage.
For MUSICA IASI data we developed a data compression tool using singular value decompositions to reduce the size of retrieval matrices. With this, the size of the orbit files reduces by 60% [3].

Tab. 1*: Required disk space for the MUSICA IASI retrieval data for the year 2017.*

Retrieval results $(H_2O, \delta D, CH_4, N_2O, HNO_3)$	22.9 TB
Retrieval results (compressed) $(H_2O, \delta D, CH_4, N_2O, HNO_3)$	9.2 TB
A posteriori evaluation $(only\ \{H_2O, \delta D\} - pairs)$	6.6 TB

Towards a data driven analysis

Data mining techniques are useful for characterizing large datasets and identifying structures in the data.
As a first step towards a data driven analysis for the MUSICA IASI data, we apply the clustering algorithm HDBSCAN [4] to the 4-dimensional distribution of ($H_2O, \delta D, latitude, longitude$). A more general approach for also considering the temporal dimension is shown in [5].
Future plans are to attribute these statistically derived clusters to underlying physical processes.

Ongoing projects

MOTIV *(collab. with ETH Zurich, FU Berlin)*
- Establishing water isotopologue measurements (IASI, NDACC) for tagging moisture pathways and processes
- Supported by simulations of isotope-enabled models ICON-ART-Iso (global, nonhydrostatic) [2] and COSMO-iso (regional, nonhydrostatic) [6]

TEDDY *(collab. with University of Tokyo)*
- Assimilation of IASI data (2016 – 2018) into the model IsoGSM [7] as observational proxy for latent heat exchange
- Assessment of potential to improve NWP skills

ESA S5p+I H2O-ISO *(collab. with University of Leicester and University of Bergen)*
- Performing H2O/HDO retrievals from the TROPOMI sensor onboard the satellite Sentinel-5p for the period 2018-2019
- Validation with NDACC and TCCON data
- development of a combined IASI+S5p product with the objective of detecting $\{H_2O, \delta D\}$ – pairs in the boundary layer independently from the free troposphere

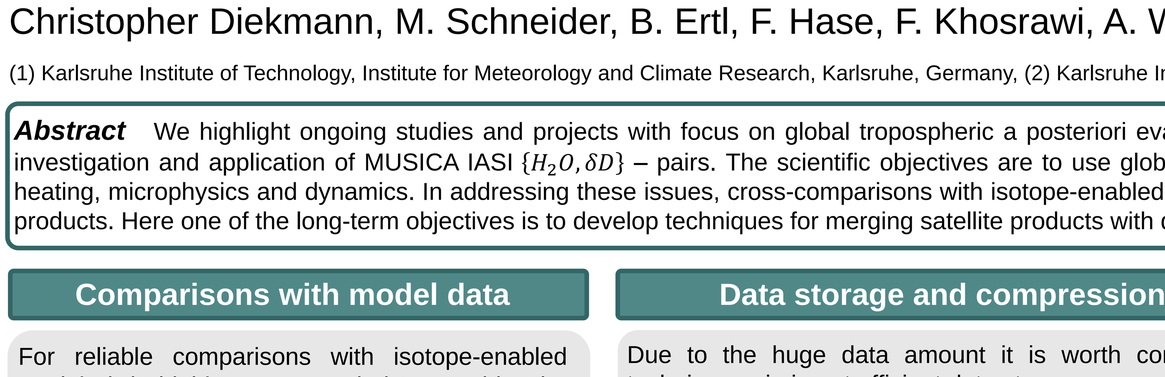

Fig. 1: *$\{H_2O, \delta D\}$ – pair distributions obtained from ECHAM-wiso simulations as original model output sampled for IASI overpasses at 5km (left), as processed according to the IASI sensitivities (middle) and from IASI retrievals (right). The colored contour lines mark the areas that contain 66% of all $\{H_2O, \delta D\}$ – pairs. The black dashed lines represent Rayleigh curves corresponding to different initialisation conditions and atmospheres (Figure adapted from [1]).*

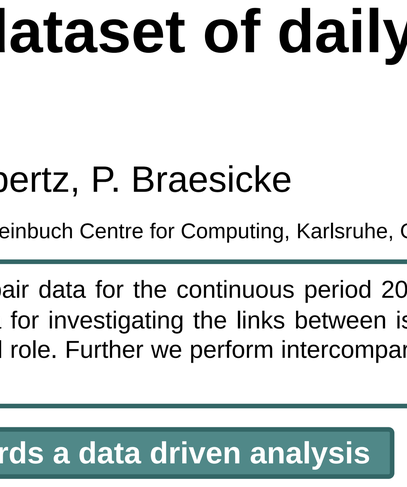

Fig. 2: *Identification of density-based clusters including events that are collocated in the two-dimensional {lat, lon} – space (top panel) as well as in the {H_2O, δ D} – space (bottom panel). The density-based clustering algorithm HDBSCAN has been used. Data are chosen for a single IASI snapshot (evening overpasses of 01.08.2016, at 4.2km).*

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