The comprehensive multi-annual MUSICA IASI dataset of daily global free tropospheric \( \{ \text{H}_2\text{O}, \delta\text{D}\} \)-pairs: demonstration

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Abstract

We present the new MUSICA (Multi-platform remote Sensing of isotopologues for investigating the Cycle of Atmospheric water) IASI tropospheric \( \{ \text{H}_2\text{O}, \delta\text{D}\} \)-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 (\( \text{H}_2\text{O}\) and \( \text{D}_2\text{O}\)) 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 \( \{ \text{H}_2\text{O}, \delta\text{D}\} \)-pairs for the continuous period 2016 - 2018 with best sensitivities at 780 - 540 hPa (\( \approx 2.5 - 5 \) km).

The Metop IASI mission

<table>
<thead>
<tr>
<th>Sensor type</th>
<th>Measurements</th>
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<tbody>
<tr>
<td>nadir, thermal infrared</td>
<td>90,000 spectra per orbit</td>
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<tr>
<td>14 orbits per day and satellites</td>
<td>currently two satellites: 2.5 Mc spectra per day</td>
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Global coverage: twice per day; overpasses at 9:30 and 21:30 local time.

Pixel size at nadir: 12 km.

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 \( \text{H}_2\text{O}, \text{D}_2\text{O}, \text{CH}_4, \text{N}_2\text{O} \) and \( \text{HNO}_3 \)

3. a posteriori evaluation
   - quality scaling for good sensitivity with respect to \( \{ \text{H}_2\text{O}, \delta\text{D}\} \)-pairs
   - \( \approx 20\% \) (\( +0.5\) Mio. reliable \( \{ \text{H}_2\text{O}, \delta\text{D}\} \)-pair observations per day)

The comprehensive multi-annual MUSICA IASI dataset of daily global free tropospheric \( \{ \text{H}_2\text{O}, \delta\text{D}\} \)-pairs: applications


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Abstract

We highlight ongoing studies and projects with focus on global tropospheric and posteriori evaluated \( \{ \text{H}_2\text{O}, \delta\text{D}\} \)-pair data for the continuous period 2016 - 2018. Several international projects involve the investigation and application of MUSICA IASI \( \{ \text{H}_2\text{O}, \delta\text{D}\} \)-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.

Comparison of 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 \( \{ x \} \) to the atmospheric state \( \{ \text{a} \} \) is described by the averaging kernel \( \{ k \} \) as:

\[ \{ x \} = \{ A \} \{ x \} \]

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 \( \{ \text{b} \} \) that reflects how the IASI sensor would observe the modeled atmosphere. \( \{ A \} \) is calculated based on radiative transfer calculations with the Community Radiation Transfer Model (CRTM).

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\% \(^{[3]}\).

\( \text{Retrieval results:} \)

\( \{ \text{H}_2\text{O}, \text{D}_2\text{O}, \text{CH}_4, \text{N}_2\text{O} \}, \text{HNO}_3 \}

\( 22.9 \text{ TB} \)

\( \text{Retrieval results (compressed):} \)

\( \{ \text{H}_2\text{O}, \text{D}_2\text{O}, \text{CH}_4, \text{N}_2\text{O} \}

\( 9.2 \text{ TB} \)

\( \text{Posteriori evaluation (only \{H}_2\text{O}, \delta\text{D}\} - pairs) \)

\( 6.6 \text{ TB} \)

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 \( \{ \text{H}_2\text{O}, \text{D}_2\text{O}, \text{latitude}, \text{longitude} \} \). A more general approach for also considering the temporal dimensions is shown in Fig. 5. Future plans are to attribute these statistically derived clusters to underlying physical processes.

Ongoing projects

**MOTIV** (collab. with ETH Zurich, FZ Berlin)
- Estimating 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) \(^{[8]}\)

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

**ESA 6Sp+ 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-6Sp product with the objective of detecting \( \{ \text{H}_2\text{O}, \delta\text{D}\} \)-pairs in the boundary layer independently from the free troposphere