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

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1: MUSICA IASI products
2: Combination of IASI and TROPOMI products
   - Method
   - Example 1: methane
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See also: https://doi.org/10.5194/amt-2021-31
MUSICA IASI products

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

Code: PROFFIT-nadir; different retrieval products: H₂O, δD, N₂O, CH₄, and HNO₃

Spectra and Jacobians

Full state averaging kernels

Retrieval

H₂O

N₂O

CH₄

HNO₃

Temperature

Surface

Water vapor spectroscopy

Line intensity (+5%)

Line broadening (+5%)

Continuum (+10%)

Simulation

Measurement

Meas.-Simu.
MUSICA IASI products

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

Time series over Karlsruhe

Overpasses 20160627

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

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

Example of MUSICA IASI fiducial referencing: δD

H2O [ppmv]
at 3.6 km a.s.l.
N2O [ppbv]
at 11 km a.s.l.
CH4 [ppbv]
at 22 km a.s.l.
HNO3 [ppbv]
year
Method: updating a MUSICA IASI profile product with information from a TROPOMI total column product

Data assimilation formalism:

\[ x^a = x^b + G[y - Hx^b] \]
\[ G = S^b H^T [HS^b H^T + S_\epsilon]^{-1} \]

**Input**

- \( x^b \): background state vector
  - \( \rightarrow \) MUSICA IASI profile product
- \( S^b \): background state error covariances
  - \( \rightarrow \) MUSICA IASI a posteriori covariances
- \( y \): measurement state vector
  - \( \rightarrow \) TROPOMI total column product
- \( H \): measurement forward operator
  - \( \rightarrow \) TROPOMI total column kernel
- \( S_\epsilon \): measurement state error covariances
  - \( \rightarrow \) TROPOMI total column noise

**Output:**

- \( x^a \): analysed state vector
- \( G \): Kalman gain matrix

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.

Differences between the IASI and TROPOMI total columns will have the strongest impact in the lower troposphere.
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 XCH₄

TROPOMI

MUSICA IASI

Combined

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

**Problem**: we need an analytic framework for ratio remote sensing data

**Solution (developed during MUSICA)**:

1. transfer the problem to the logarithmic scale: \( \frac{\partial \ln x}{\partial x} = \frac{1}{x} \partial x \)
2. use proxy state: \( \ln \frac{\tilde{x}_{\text{HDO}}}{\tilde{x}_{\text{H2O}}} = \ln \tilde{x}_{\text{HDO}} - \ln \tilde{x}_{\text{H2O}} \)

**Transformation**:

(H2O, HDO) state
→ (H2O, δD) proxy-state

\( A_p = P A_{\log} P^{-1} \).

Transformation matrix P for (H2O, δD) proxy-state:

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

**Kernel**: \( A \)

**Proxy kernel**: \( A_p \)
... analytic framework for ratio remote sensing data

**Extension to column products:**

$$a_p^T = P_X M_X^{-1} H_{\bar{X}}^{-1} a^T H M P^{-1},$$

with

$$H = \begin{pmatrix}
    h_1 & \cdots & 0 & 0 & \cdots & 0 \\
    \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
    0 & \cdots & h_N & 0 & \cdots & 0 \\
    0 & \cdots & 0 & h_1 & \cdots & 0 \\
    \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
    0 & \cdots & 0 & 0 & \cdots & h_N \\
\end{pmatrix},
\quad
H_{\bar{X}} = \begin{pmatrix}
    \sum_{i=1}^N h_i & 0 & 0 \\
    0 & \sum_{i=1}^N h_i & 0 \\
\end{pmatrix},
\quad
M_X = \begin{pmatrix}
    \bar{X}_{H2O} & 0 \\
    0 & \bar{X}_{HDO} \\
\end{pmatrix},
\quad
P_X = \begin{pmatrix}
    +0.5 & +0.5 \\
    -1.0 & +1.0 \\
\end{pmatrix}.$$
Example 2: Combination, effect on the averaging kernels

Here we use the X6D TROPOMI product of UoL-FP v0.9.4.

Proxy averaging kernels

MUSICA IASI retrieval

MUSICA IASI retrieval with TROPOMI “assimilated”

Comparison, column kernels

Comparison, column kernels

Here we use the X6D TROPOMI product of UoL-FP v0.9.4.
Example 2: Validation of surface-near data product

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

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 X$\delta$D. 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!

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