

IASI for Surveying Methane and Nitrous Oxide in the Troposphere: MUSICA products and its validation

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 - I. General retrieval characteristics
 - II. A posteriori calculated difference between CH₄ and N₂O
2. Theoretical Characterisation
 - I. Representativeness
 - II. Error Assessment
3. Validation by using a Multi-Platform Reference Database
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 - II. GAW in situ, and NDACC/FTIR
4. A posteriori CH₄ Correction
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1. Remote sensing of CH_4 and N_2O

General Retrieval Characteristics

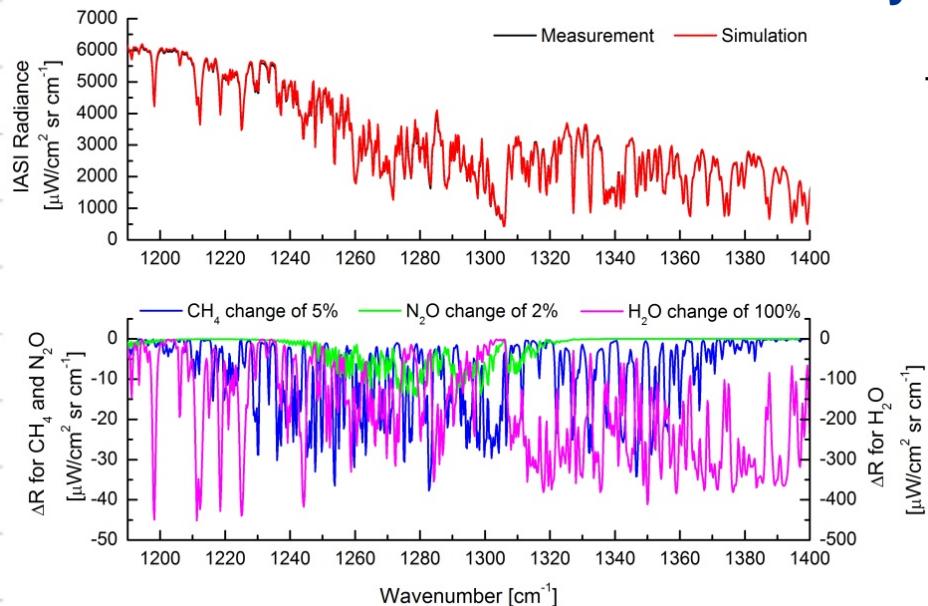
IASI processor developed during the ERC project MUSICA (**M**ULTi-platfrom remote **S**ensing of **I**sotopologues for investigating the **C**ycle of **A**tmospheric water), based on the retrieval code PROFFIT-nadir [Schneider and Hase, 2011]

Optimal estimation retrieval: combine a priori information with the measured IASI spectra and estimate the most likely atmospheric state.

A priori information is kept constant (no variation in space and time), i.e., all the retrieved variability is introduced by the IASI spectra.

Simultaneous retrieval of H_2^{16}O , HD^{16}O , CH_4 , N_2O and HNO_3 (+ CO_2), atmospheric and skin temperature on log. scale.

Key!!



The spectral signatures of H_2O variations are more than an order of magnitude stronger than the signatures of CH_4 and N_2O



Quality of CH_4 and N_2O products strongly depends on a correct interpretation of H_2O interferences

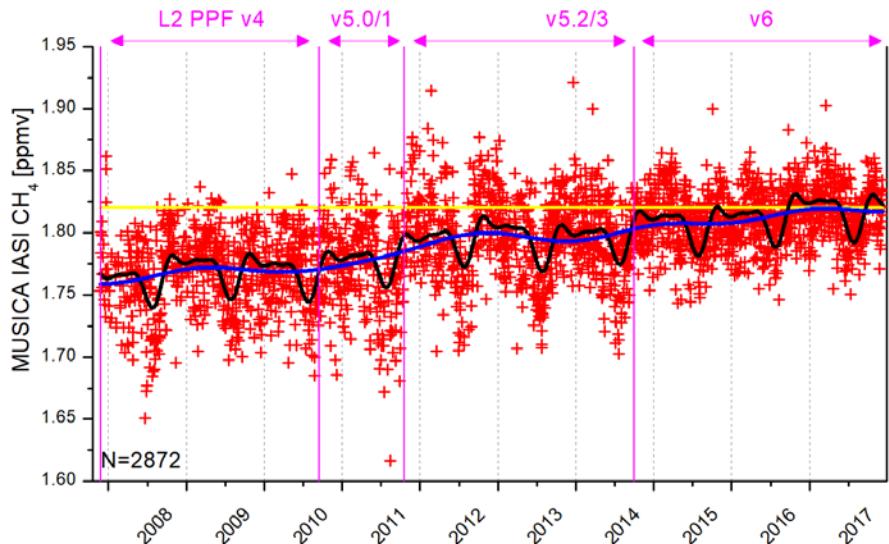


MUSICA IASI incorporates a sophisticated H_2O isotopologue retrieval and water continuum contributions (MT_CKD v2.5.2)

1. Remote sensing of CH₄ and N₂O

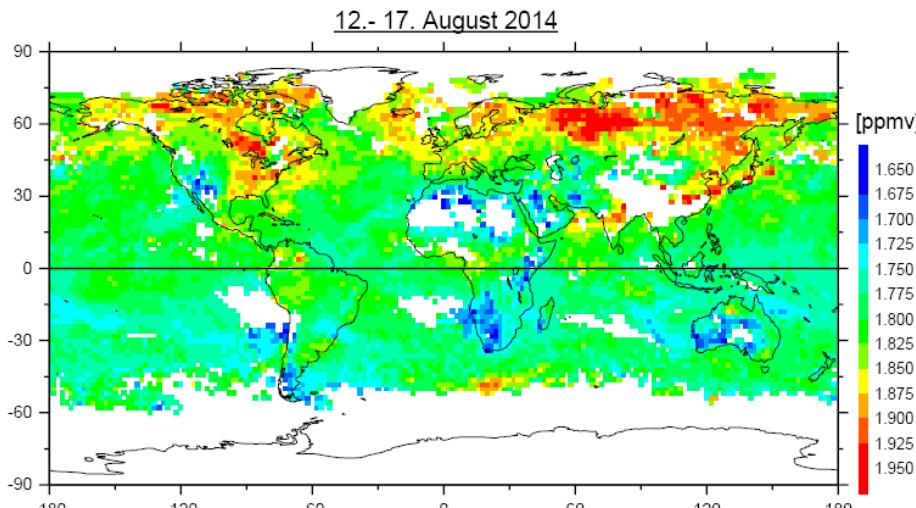
Long-term monitoring

Example of continuous time series of MUSICA IASI CH₄ daily mean data retrieved at 4.2 km altitude in the surroundings of Tenerife Island between 2007 and 2017.



Global coverage

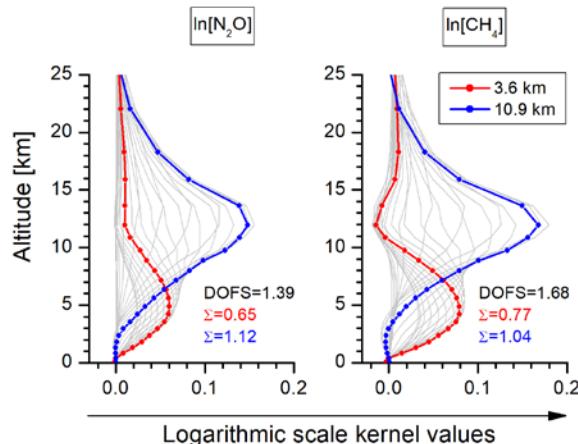
Example of global geographical distribution of the free tropospheric MUSICA IASI CH₄ product retrieved at 4.2 km altitude, filtered for $c_{\text{sen}} < 50\%$ and averaged for an latitude x longitude area of $2^{\circ} \times 2^{\circ}$.



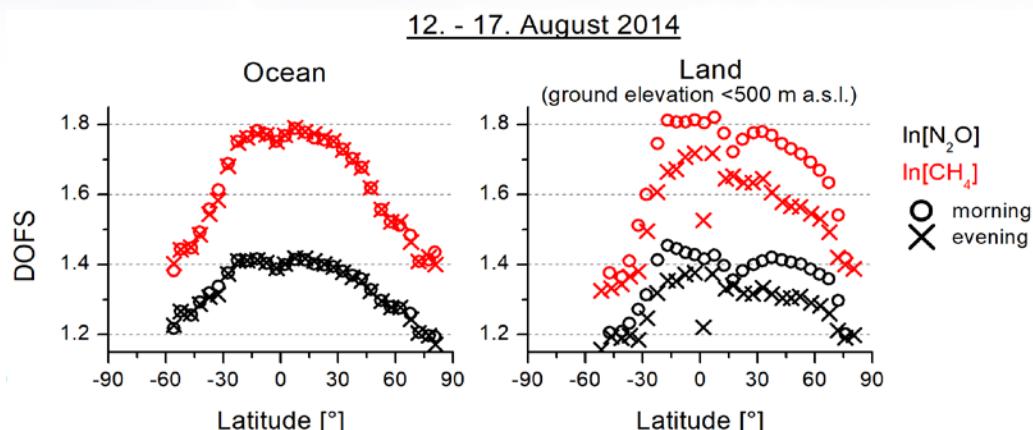
IASI has a great potential for CH₄ and N₂O monitoring and for greenhouse gas cycle studies

2. Theoretical Characterisation

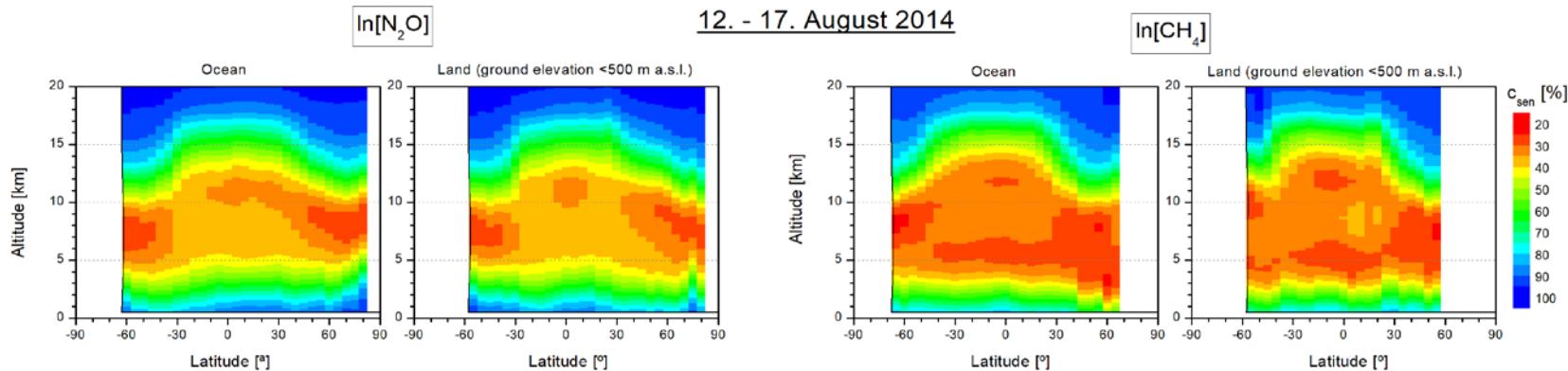
Example for mid-latitude summer land pixel



Representativeness: Averaging Kernels

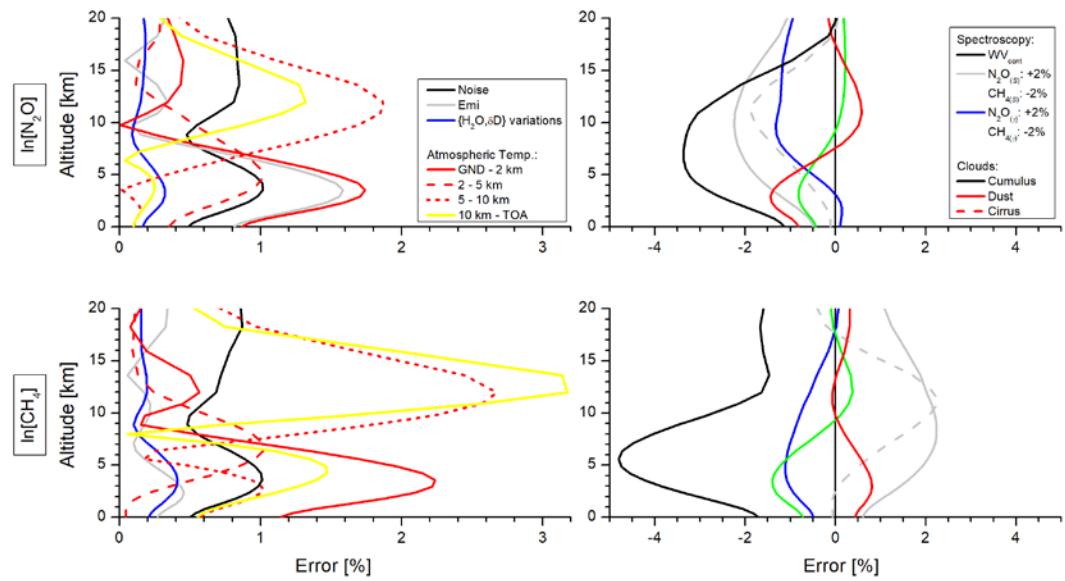


- ✓ Altitude regions that well-detectable by MUSICA IASI products: $c_{sen} < 50\%$
- ✓ MUSICA IASI products can capture atmospheric variations of CH_4 and N_2O between 2-16 km with a vertical resolution of 5-8 km
- ✓ MUSICA IASI CH_4 data offer a better sensitivity than N_2O data



2. Theoretical Characterisation

Example for mid-latitude summer land pixel



Error Assessment

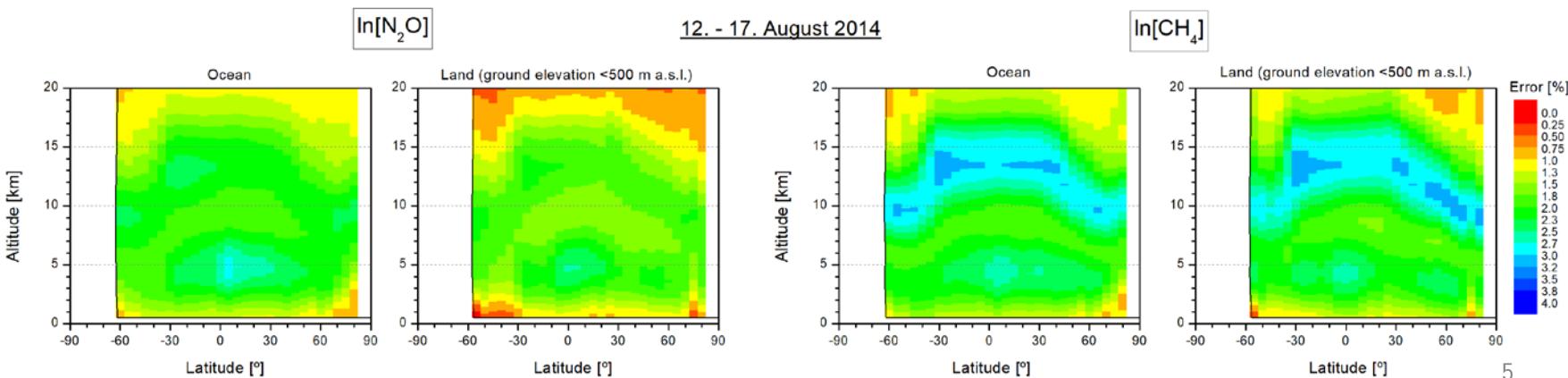
Statistical sources (Gaussian distribution):

- ✓ Measurement noise < 1%
- ✓ Emissivity < 0.5%
- ✓ H₂O cross-dependency < 0.5%
- ✓ **Atmospheric temperature ~ [0-3]%**

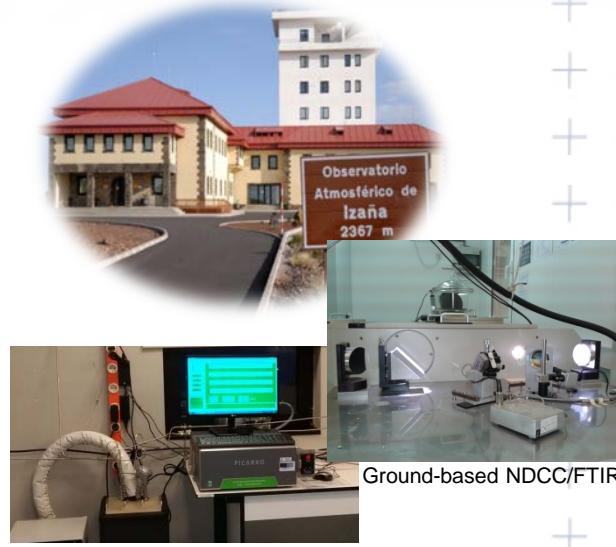
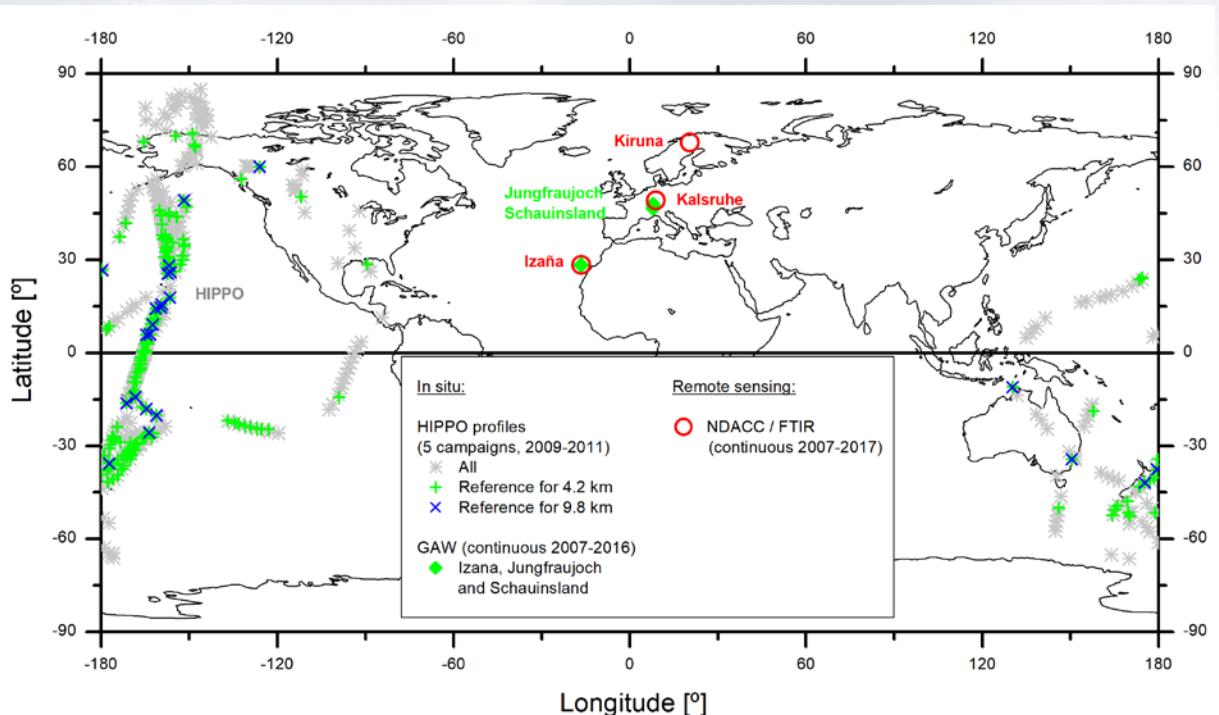
Non-Gaussian sources:

- ✓ Spectroscopy ~ [-2, 2]%
- ✓ Water continuum ~[-1,0]%
- ✓ **Clouds ~[-4.5, 1]%**

Latitudinal Cuts of Leading Errors (atmospheric temperature and measurement noise)



3. Validation by using a Multi-Platform Database



HIPPO (HIAPER Polo-to-Pole Observation) aircraft profiles

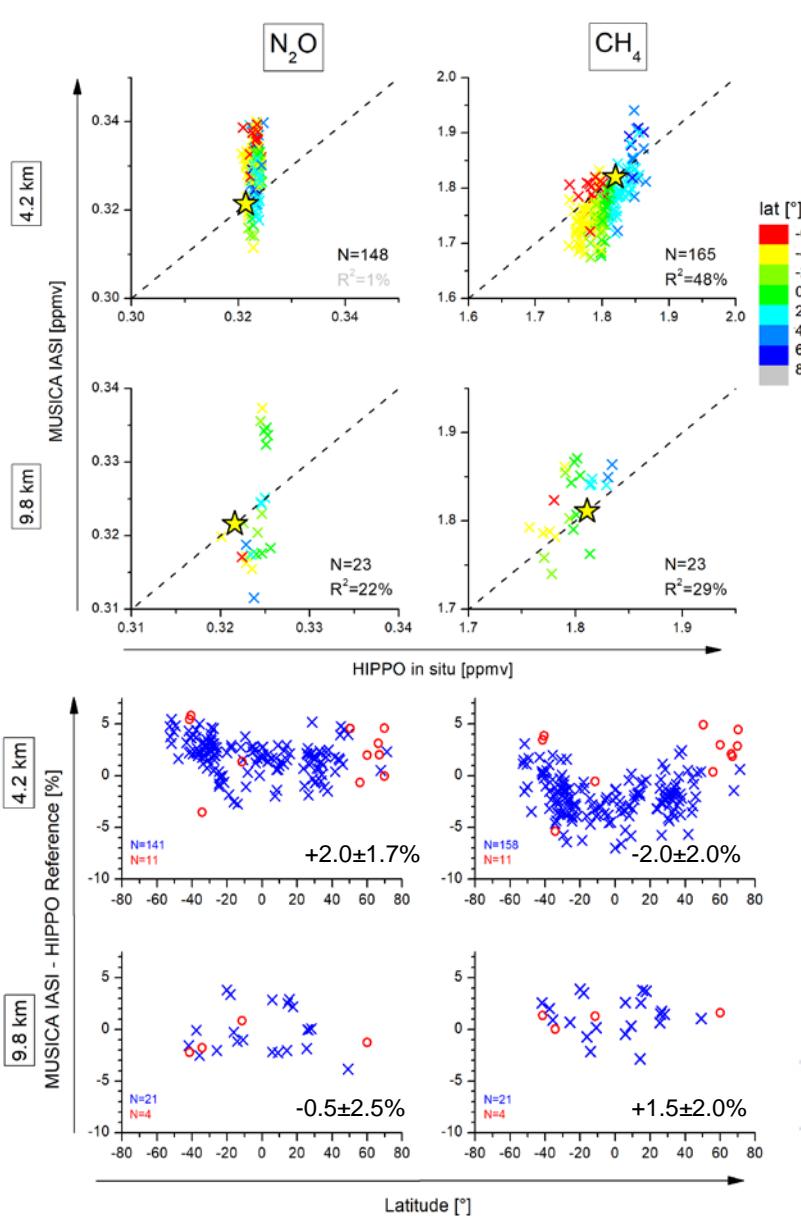
- High precision&accuracy, high vertical resolution, good latitudinal coverage (67°S - 80°N , Pacific Ocean)
- Accuracy, precision, profiling capability and latitudinal gradients**

GAW (Global Atmospheric Watch) in situ and NDACC/FTIR (Fourier Transform Infrared Spectrometer)

- High precision&accuracy, continuous (GAW), quasi continuous (daytime, FTIR), long-term series
- Precision, profiling capability and temporal signals that are detectable**

[Details on collocation, data treatment and filtering are given in Extra Material slides]

3. Validation by using a Multi-Platform Database

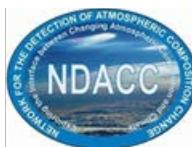
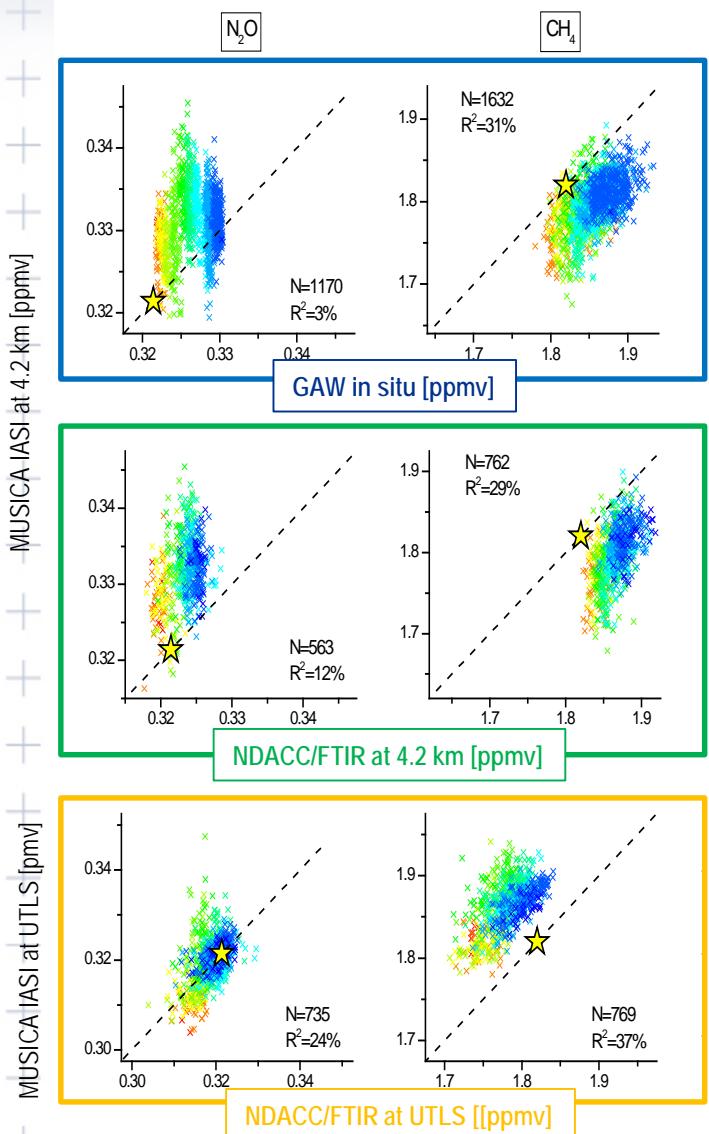


HIPPO1 (January 2009)
 HIPPO2 (November 2009)
 HIPPO3 (March/April 2010)
 HIPPO4 (June 2011)
 HIPPO5 (August/Sep 2011)

- ✓ MUSICA IASI data capture well CH_4 latitudinal gradients, but not for N_2O (very small variations).

- ✓ Latitudinal dependency of bias (according to IASI sensitivity).
- ✓ Precision: 1.5-2.5%
- ✓ Accuracy: $\pm 2\%$

3. Validation by using a Multi-Platform Database



Tenerife, 28°N, 2007-2017
Karsruhe, 49°N, 2010-2017
Kiruna, 68°N, 2007-2017

- ✓ GAW and NDACC/FTIR comparison confirms the HIPPO results over time.
- ✓ The overall precision: 1-2% for N_2O and 1-3% for CH_4 (free troposphere and UTLS).

But, what temporal signals are really detectable by the MUSICA IASI products?

Temporal decomposition of a time series into signals belonging to different timescales:

$$x(t) = \underbrace{\overline{x_m([t_1, t_2])}}_{\text{Reference value}} + s(t) + l(t) + d(t)$$

↓ Day-to-Day variations
 ↓ Long-term signal
 ↓ Seasonal cycle

[Comparison for Karlsruhe and Kiruna is shown in Extra Material slides]

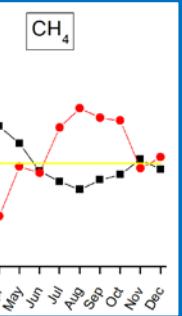
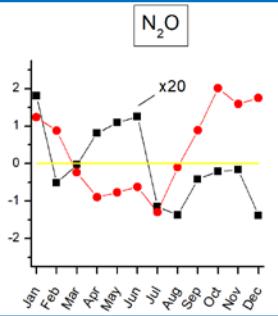
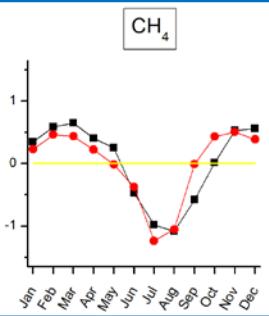
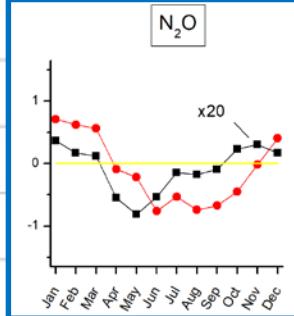
3. Validation by using a Multi-Platform Database

Seasonal cycle relative to long-term background [%]

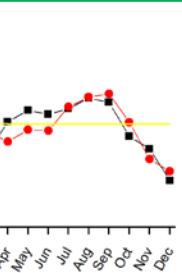
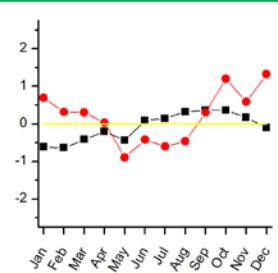
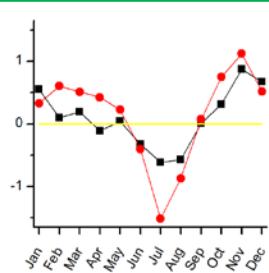
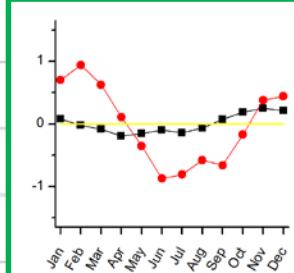
Tenerife, 28°N, 2007-2017

Karlsruhe, 49°N, 2010-2017

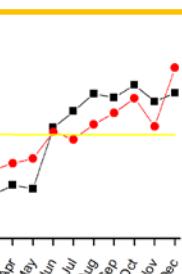
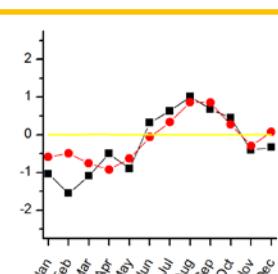
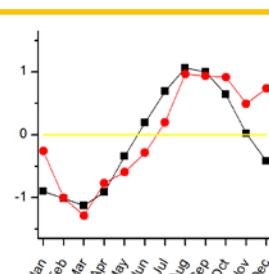
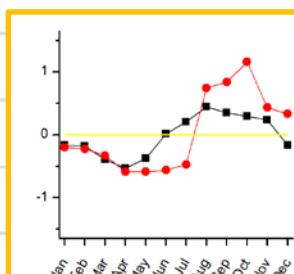
GAW in situ



NDACC/FTIR at 4.2 km



NDACC/FTIR at UTLS

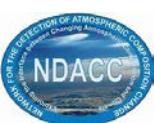


MUSICA IASI red, GAW and NDACC/FTIR black

Temporal Decomposition

$$x(t) = \bar{x}_m([t_1, t_2]) + s(t) + l(t) + d(t)$$

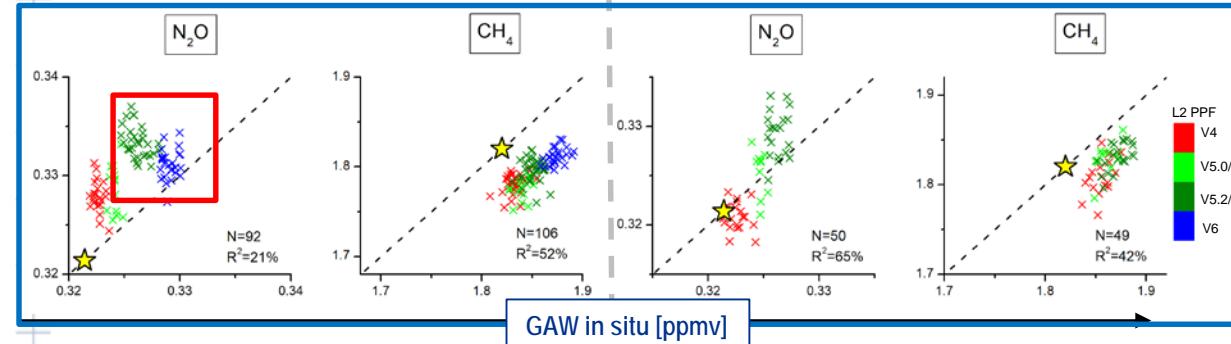
- ✓ MUSICA IASI data capture well the CH₄ seasonal cycles (phase and amplitude) at free troposphere only at subtropical latitudes.
- ✓ Not for N₂O (very small variations in free troposphere).
- ✓ For all latitudes and for both N₂O and CH₄ MUSICA IASI data capture well the seasonal cycles (phase and amplitude) in the UTLS.



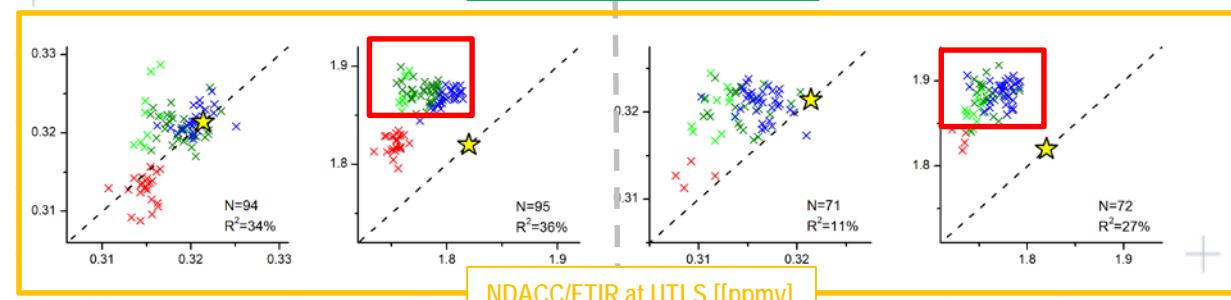
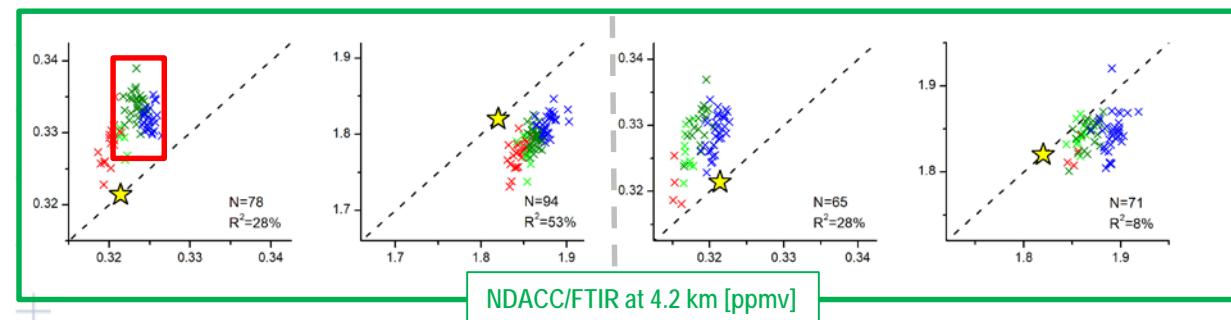
3. Validation by using a Multi-Platform Database

Long-term signals: Deseanolised monthly mean

Tenerife, 28°N, 2007-2017



Karlsruhe, 49°N, 2010-2017



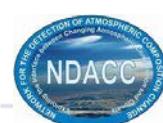
Temporal Decomposition

$$x(t) = \overline{x_m([t_1, t_2])} + s(t) + l(t) + d(t)$$

- ✓ MUSICA IASI data are affected by an inconsistency between the versions EUMETSAT L2 PPF v5.2/3 and V6 (used as a priori information).
- ✓ When this inconsistency is not considered (Karlsruhe) the agreement with GAW in situ suggests that MUSICA IASI data detects the long-term variations in the free troposphere up to mid-latitudes.

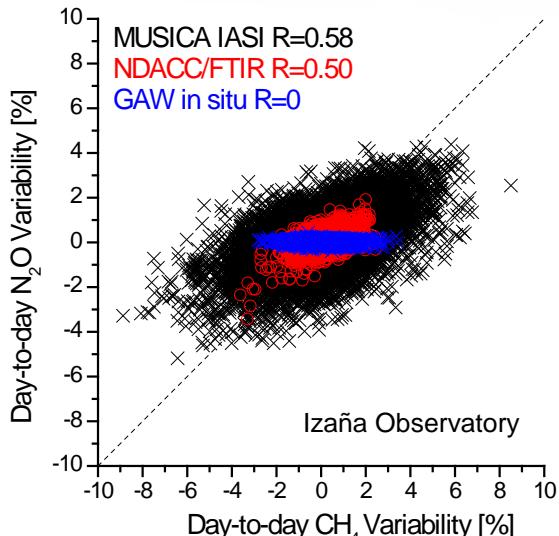


GLOBAL
ATMOSPHERE
WATCH



4. A posteriori CH_4 Correction

A posteriori calculated difference between CH_4 and N_2O



N_2O concentrations show a rather low short-term variability and their long-term increase is very stable



Significant variations in the N_2O retrievals are due to errors

Assuming that N_2O and CH_4 have correlated errors (e.g. temperature, clouds,...) and common signals (e.g. UTLS shift)



Combining co-retrieved N_2O and CH_4 to generate a combined product with reduced errors and common signals, and then better representativeness of sources/sinks signals

$$\hat{x}_{\text{CH}_4} - \hat{x}_{\text{N}_2\text{O}} = \underbrace{x_{a,\text{CH}_4} - x_{a,\text{N}_2\text{O}}}_{\text{Retrieved states}} + \underbrace{\mathbf{A}_{\text{CH}_4}(x_{\text{CH}_4} - x_{a,\text{CH}_4}) - \mathbf{A}_{\text{N}_2\text{O}}(x_{\text{N}_2\text{O}} - x_{a,\text{N}_2\text{O}})}_{\text{A priori}} + \underbrace{\Delta x_{\text{CH}_4} - \Delta x_{\text{N}_2\text{O}}}_{\text{Difference of errors is smaller than individual errors}}$$

↓ ↓

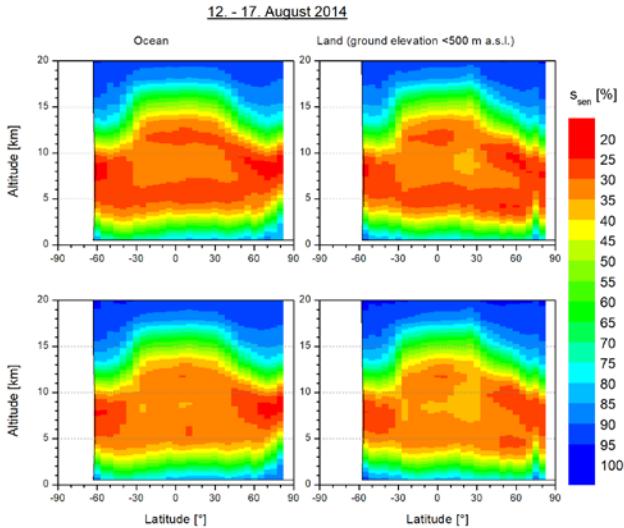
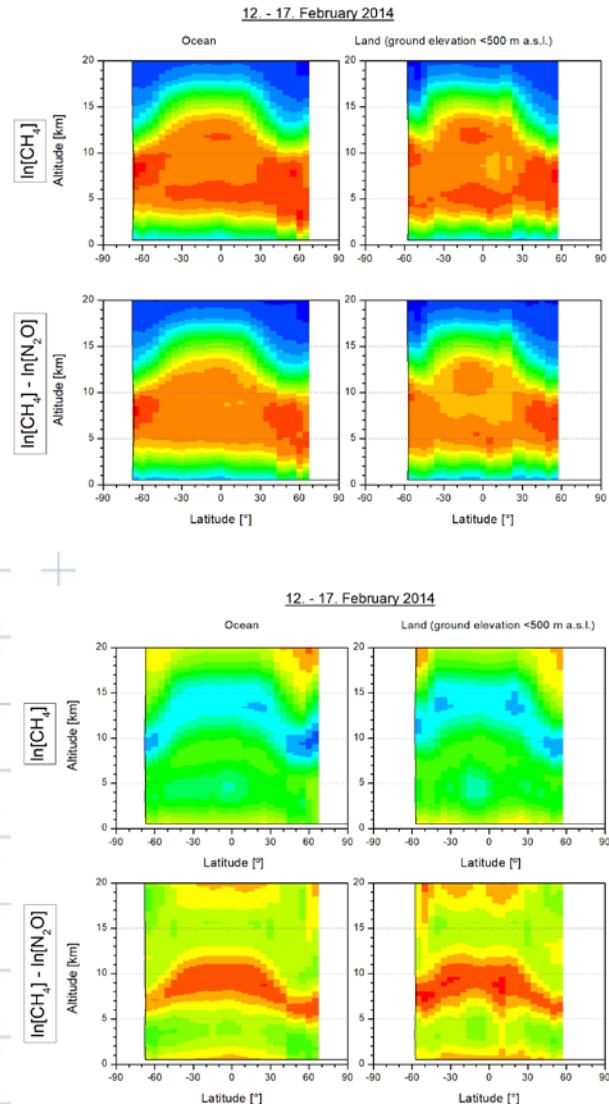
Averaging kernels

We propose two approaches for calculating the combined products based on:

(1) N_2O model simulations (CH_4^*) and (2) N_2O climatology (CH_4') (details on Extra Material slides).

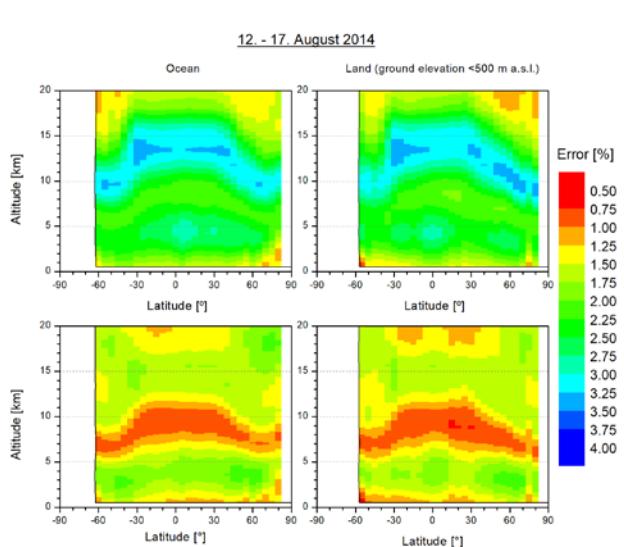
But, both can be characterised by the $\{\ln[\text{CH}_4] - \ln[\text{N}_2\text{O}]\}$ state.

4. A posteriori CH_4 Correction



Sensitivity

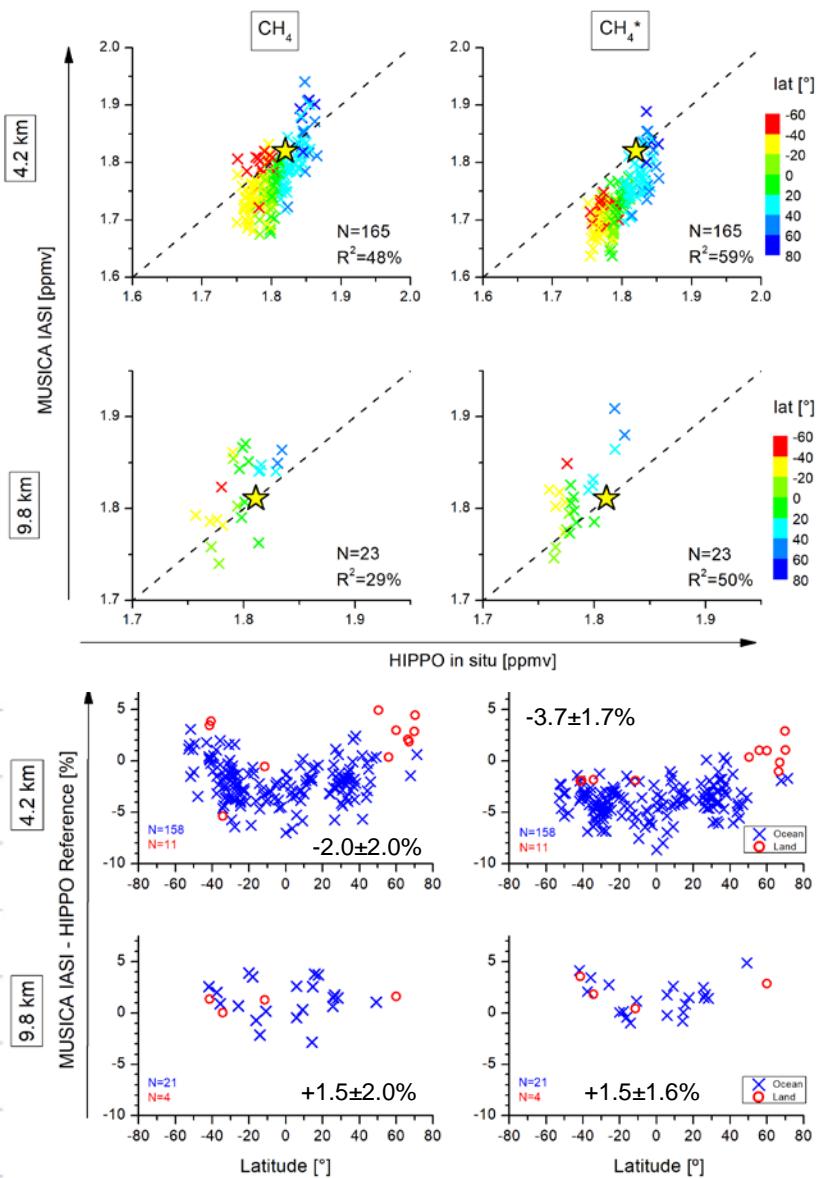
Similar vertical distribution, but slightly lower sensitivity for the combined product



Leading Errors

The a posteriori CH_4 correction with co-retrieved N_2O offers better precision!!!

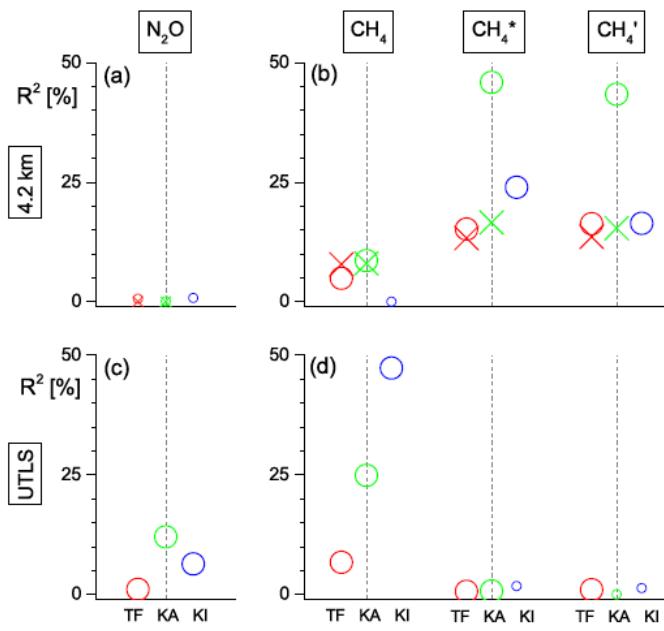
4. A posteriori CH₄ Correction



- ✓ Better estimation of latitudinal gradient
- ✓ High precision



$$x(t) = \overline{x_m([t_1, t_2])} + s(t) + l(t) + d(t)$$



5. Summary and Outlook

- ✓ The MUSICA IASI data capture signals that are larger than 1-2%, like the latitudinal gradients, the long-term increase and the seasonal cycles in the UTLS region.
- ✓ While for N_2O the sensitivity is mainly limited to the UTLS region, for CH_4 at low latitudes the MUSICA IASI processor can detect variations that take place in the free troposphere independently from the variations in the UTLS region.
- ✓ Room for improvements, but the benefits are limited (other sophisticated retrievals point out the same results, e.g. rough profile capability only for lower and middle latitudes).

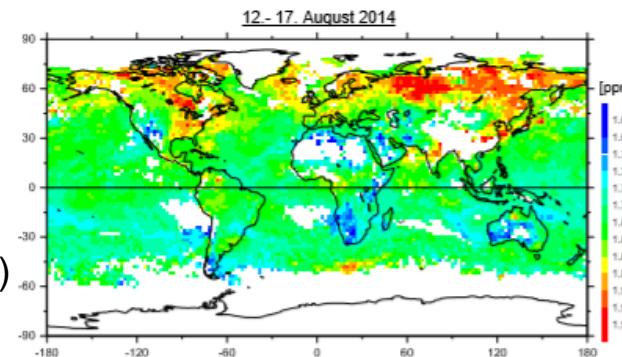
Our next plans:

(1) Performing retrievals for many orbits

(producing data globally for longer time periods)

IASI A+B measures about 2.5 Millions spectra per day!

We focus on the about 10% that are cloud-free (0.25 Millions)



(2) Examining the usefulness of IASI CH_4 and N_2O data for source/sink studies

By combining IASI space-based observations and model estimates, we will investigate the kind of CH_4 and N_2O sink/source signals at a global scale that can be captured by high quality IASI observations, and the transport of the CH_4 and N_2O in the atmosphere.



Many Thanks for your Attention!!

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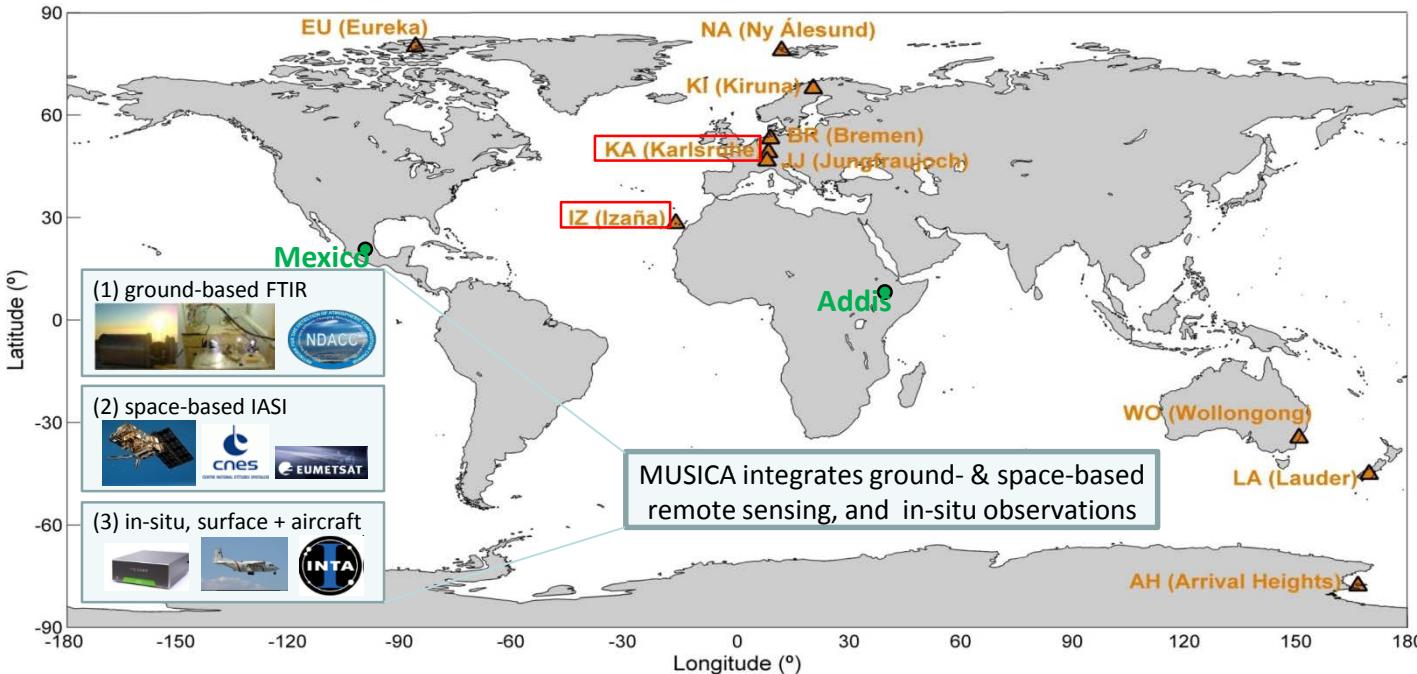
Extra Material

Project MUSICA



MULTI-platfrom remote Sensing of Isotopologues for investigating the Cycle of Atmospheric water, European Research Council, 2011-2016.

Objetive: Generating robust tropospheric $\{\text{H}_2\text{O}, \delta\text{D}\}$ pairs using ground-based NDACC/FTIR (Fourier Transform Infrared Spectrometer) and space-based MetOp/IASI (Infrared Atmospheric Sounding Interferometer).



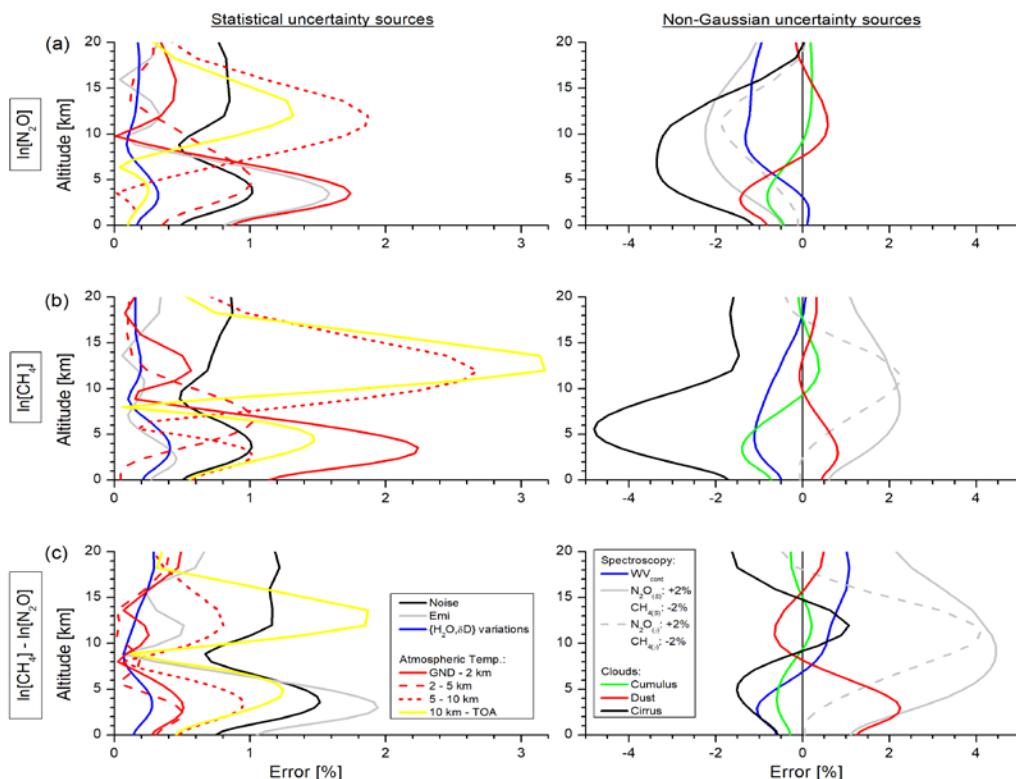
Publications: Schneider and Hase, 2011; Schneider et al., 2012; Schneider et al., 2013; Wiegele et al., 2014; Barthlott et al., 2015; Christner, 2015; Dyrroff et al., 2015; Schneider et al., 2015; González et al., 2016; Schneider et al., 2016; Barthlott et al., 2017; Borger et al., 2017; Christner et al., 2017; García et al., 2017; Schneider et al., 2017.

And more than 20 publications related with MUSICA activities.

Theoretical Characterisation (Continuation)

Assumed Uncertainties in the Error Assessment

Uncertainty Source	Uncertainty Value	Uncertainty Source	Uncertainty Value
Measurement noise	Pequignot et al. (2008)	Line intensity and pressure broadening N2O	2%
Temperature 0-2km	2K	Line intensity and pressure broadening CH4	-2%
Temperature 2-5km, 5-10km	1K	Opaque cumulus cloud	10% fractional cover with cloud top at 1.3, 3.0 and 4.9 km
Temperature above 10km	1K	Cirrus cloud	Particle properties OPAC "Cirrus3" 1km thickness, 50% fractional cover with cloud top at 6, 8, 11 and 14 km
Surface emissivity	1% at 1185, 1240, 1295, 1350, and 1405 cm ⁻¹	Mineral dust cloud	Particle properties OPAC "Desert" Homogeneous coverage for layers: ground-2 km, 2-4 km and 4-6km
Water vapour continuum	10% underestimation	{H ₂ O, δD} variations	{10%, 10%}, with 2.5km of correlation length



Error vertical profiles for a mid-latitude summer land pixel

Collocation, Data Filtering and Data Treatment

Collocation and data filtering

HIPPO:

- I. All IASI observations within $2^{\circ}\times 2^{\circ}$ latitude/longitude box around the mean location of each HIPPO profile, $\pm 12\text{h}$ around the mean time of each HIPPO profile.
- II. Altitude of HIPPO profiles: free troposphere (4.8 km) up to 8 km, for ULTS (9.8 km) up to 12.5 km

GAW&NDACC/FTIR:

- I. All IASI observations within ~ 110 km box south of GAW&NDACC/FTIR stations
- II. Night-time means (GAW in situ), $\pm 8\text{h}$ (NDACC/FTIR), evening and morning overpass (IASI)

MUSICA/IASI:

$c_{\text{sen}} < 50\%$, cloud free pixels, residual-to-signal in the fitted window < 0.004 , skin temperature $> 275\text{K}$

HIPPO Data Treatment

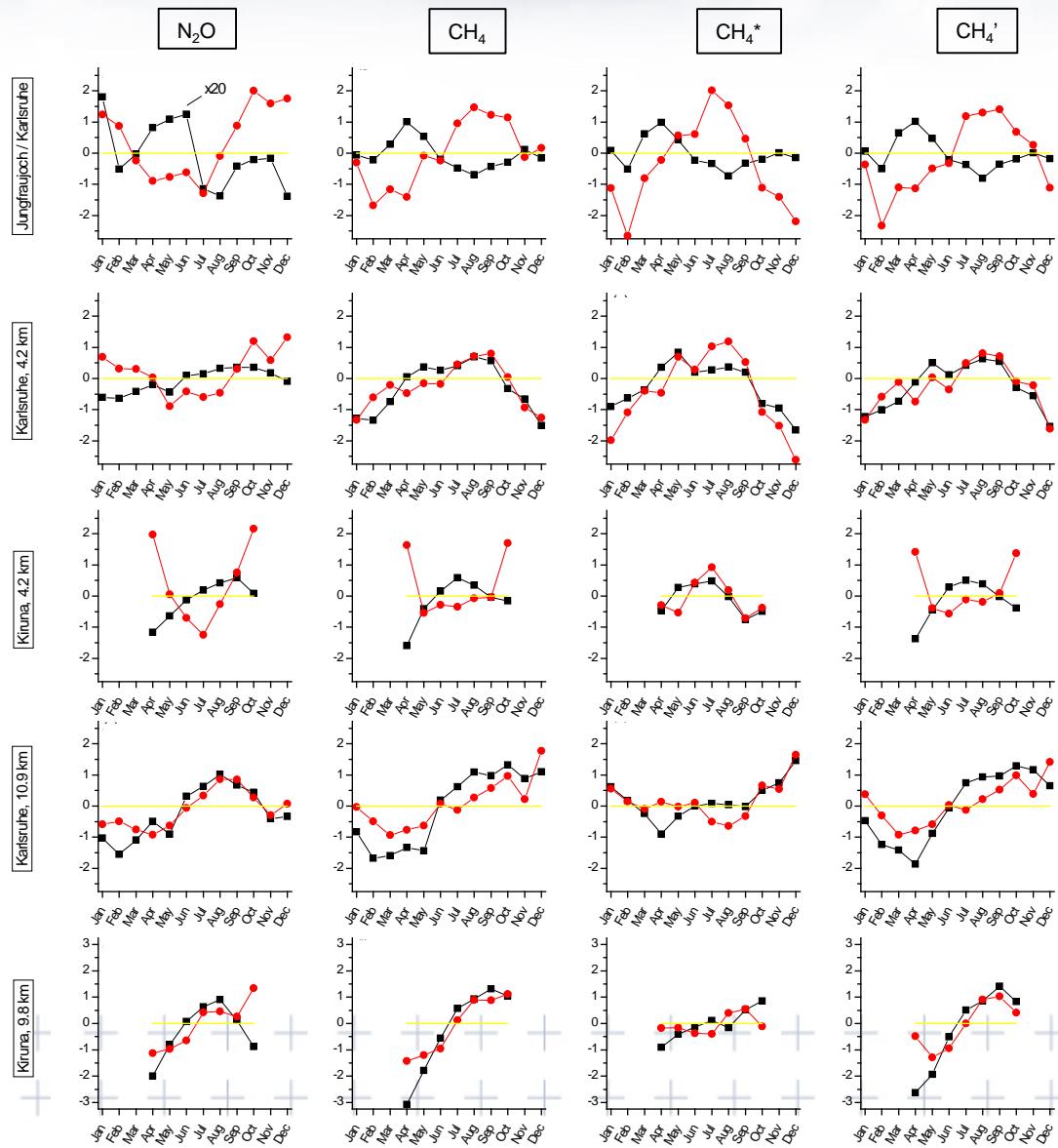
- I. The vertically highly-resolved HIPPO profiles are degraded applying the IASI averaging kernels:

$$\hat{h} = A(h - x_a) + x_a.$$
- II. The HIPPO profiles are extended by the a priori data used by the MUSICA IASI processor.

Comparison of MUSICA IASI and NDACC/FTIR remote sensing data

- I. The NDACC/FTIR data are adjusted to the unique MUSICA a priori data by adding $(A_{\text{FTIR}} - I)(x_a - x_{a;\text{FTIR}})$ to the NDACC/FTIR retrieval results (being A_{FTIR} and $x_{a;\text{FTIR}}$ the averaging kernels and a priori state corresponding to the NDACC/FTIR retrieval, respectively) [Rodgers and Connor, 2003].
- II. MUSICA IASI N_2O data are compared with smoothed NDACC/FTIR data at all altitudes. The free tropospheric MUSICA IASI CH_4 and CH_4^* data are also compared to smoothed NDACC/FTIR data. However, in the UTLS region the MUSICA IASI and NDACC/FTIR CH_4 and CH_4^* data are directly compared (no prior smoothing of the NDACC/FTIR data).

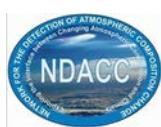
Validation by using a Multi-Platform Database (Continuation)



Temporal Decomposition

$$x(t) = \overline{x_m([t_1, t_2])} - s(t) - l(t) + d(t)$$

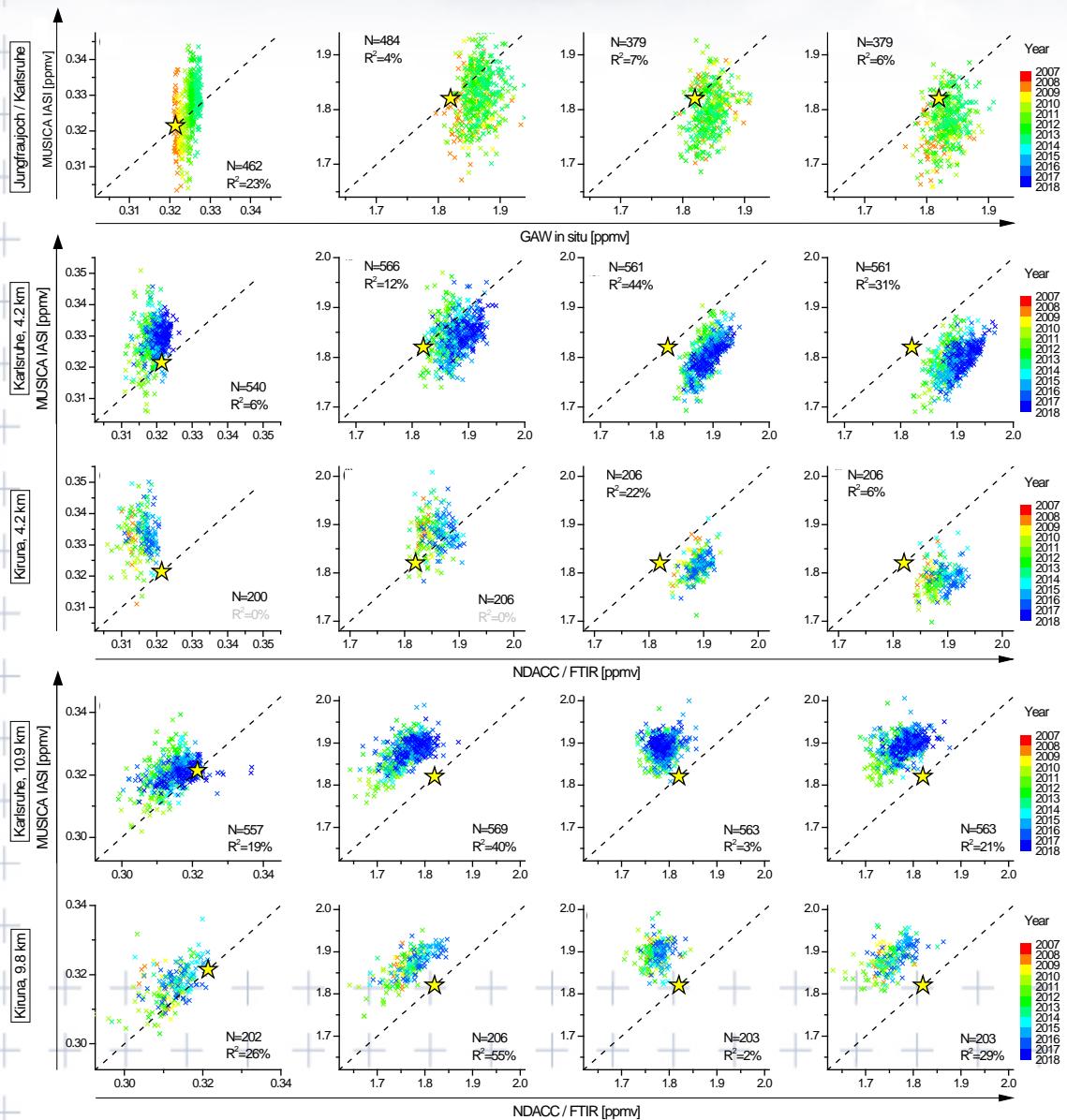
Seasonal cycle relative to long-term background [%]



Karslruhe, 49°N, 2010-2017

Kiruna, 68°N, 2007-2017

Validation by using a Multi-Platform Database (Continuation)



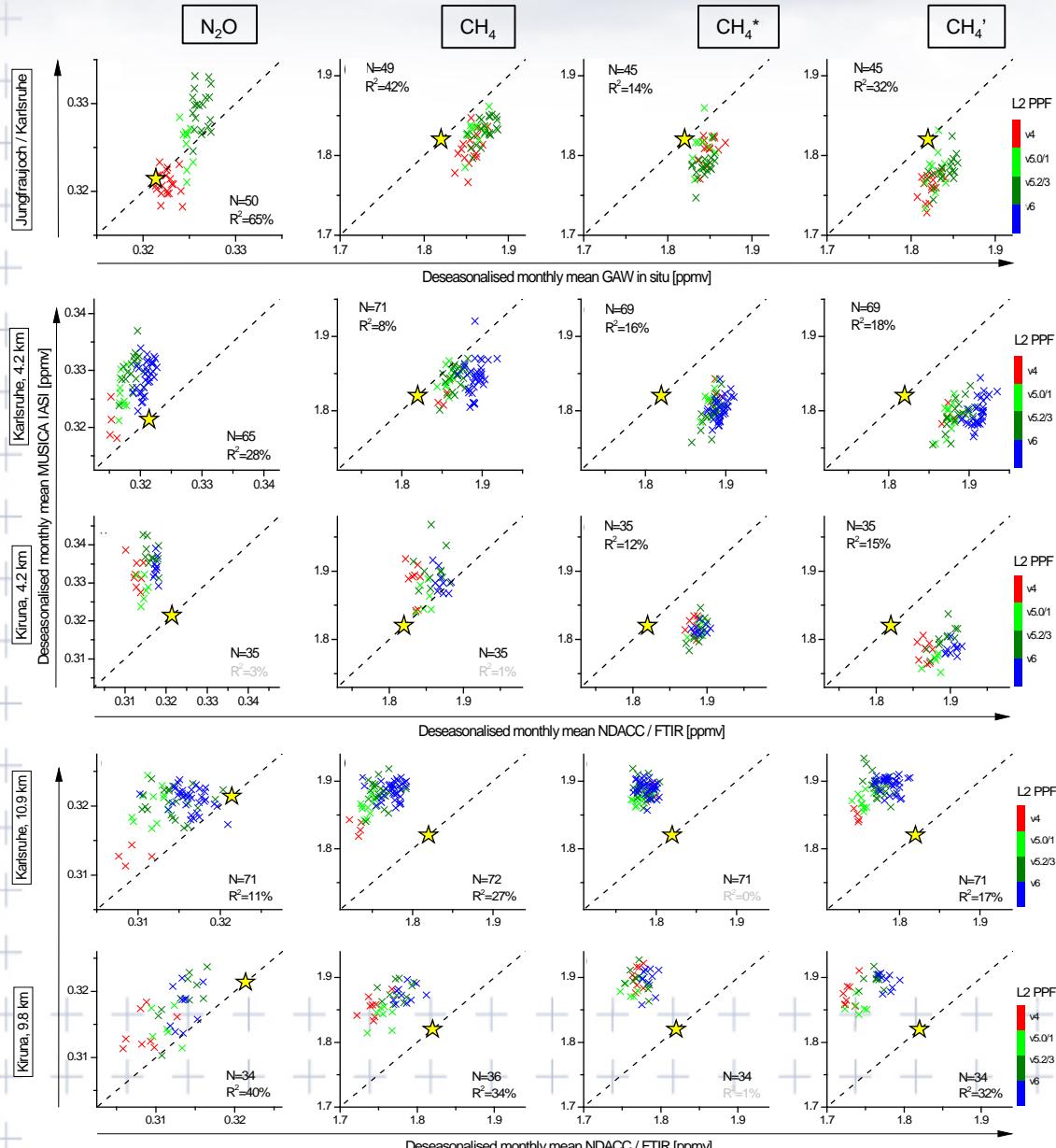
Daily Observations



Kaiserslautern, 49°N, 2010-2017

Kiruna, 68°N, 2007-2017

Validation by using a Multi-Platform Database (Continuation)



Temporal Decomposition

$$x(t) = \boxed{x_m([t_1, t_2])} + s(t) - \boxed{l(t)} - \boxed{d(t)}$$

Long-term signals:
Deseanolised montlhly mean



Karslruhe, 49°N, 2010-2017

Kiruna, 68°N, 2007-2017

A posteriori CH₄ Correction (Continuation)

(1) N₂O Model Simulations

Approach: As N₂O is very stable, the horizontal, vertical and temporal N₂O variations can be captured well by model simulations. Then, the corrected CH₄ state is:

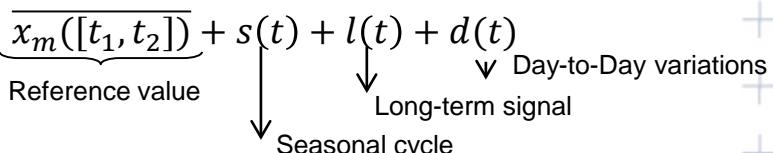
$$\hat{x}_{\text{CH}_4}^c = \underbrace{(\hat{x}_{\text{CH}_4} - \hat{x}_{\text{N}_2\text{O}})}_{\text{A posteriori calculated difference}} + \mathbf{A}_{\text{N}_2\text{O}} \underbrace{(m_{\text{N}_2\text{O}} - x_{a,\text{N}_2\text{O}})}_{\text{Model simulations}} + x_{a,\text{N}_2\text{O}}$$

But, we are interested in quantifying the errors in the corrected CH₄ products only due to errors in the MUSICA IASI retrievals, not in model simulations. Thereby, we assume $m_{\text{N}_2\text{O}} = x_{a,\text{N}_2\text{O}}$

$$\hat{x}_{\text{CH}_4}^* = (\hat{x}_{\text{CH}_4} - \hat{x}_{\text{N}_2\text{O}}) + x_{a,\text{N}_2\text{O}}$$

(2) N₂O Climatology

Approach: Temporal decomposition of a time series $x(t) = \overline{x_m([t_1, t_2])} + s(t) + l(t) + d(t)$ into signals belonging to different timescales



Assuming that seasonal and long-term CH₄ variations are well captured by MUSICA IASI CH₄ products, we only correct for short-term signals

$$\hat{x}_{\text{CH}_4}^c(t) = \hat{x}_{\text{CH}_4}(t) - \underbrace{(\hat{x}_{m,\text{N}_2\text{O}}[t_1, t_2] + \hat{x}_{d,\text{N}_2\text{O}}(t))}_{\text{Co-retrieved N}_2\text{O product}} + \mathbf{A}_{\text{N}_2\text{O}} \underbrace{(m_{\text{N}_2\text{O}}[t_1, t_2] - x_{a,\text{N}_2\text{O}})}_{\text{N}_2\text{O climatology}} + x_{a,\text{N}_2\text{O}}$$

Assuming again $\overline{m_{\text{N}_2\text{O}}[t_1, t_2]} = x_{a,\text{N}_2\text{O}}$

$$\hat{x}'_{\text{CH}_4}(t) = \hat{x}_{\text{CH}_4}(t) - \left(\hat{x}_{m,\text{N}_2\text{O}}[t_1, t_2] + \hat{x}_{d,\text{N}_2\text{O}}(t) \right) + x_{a,\text{N}_2\text{O}}$$

The correction (1) strongly depends on the quality of N₂O model simulations, while (2) not.

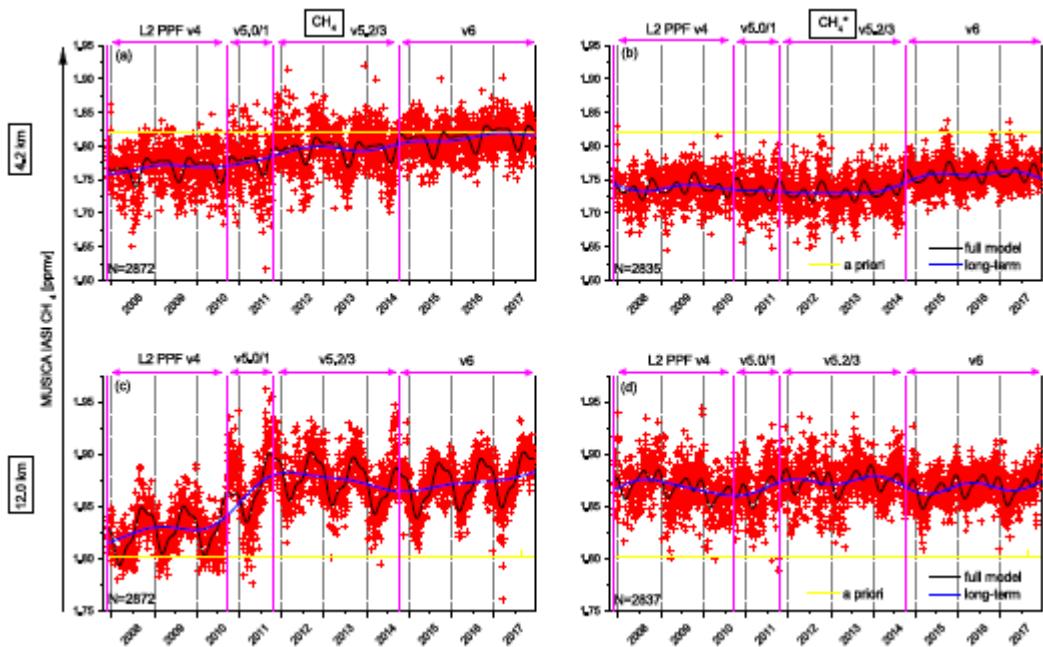
Time Series Model and Long-term Data Consistency

The modelled time series, for estimating the mean values for a reference period and for a first guess separation of seasonal cycle and long-term signals, is obtained by a multi-regression fit of different coefficients that consider variations on different timescales:

$$x_m(t) = \overline{x_m([t_1, t_2])} \longrightarrow \text{Reference value}$$

$$+ A_0 + A_1 t + \underbrace{\sum_{1 \leq i \leq \frac{\Delta t}{\Delta t}} \left\{ A_{\sin, i} \sin \left(\frac{2\pi i}{\Delta t} t \right) + A_{\cos, i} \cos \left(\frac{2\pi i}{\Delta t} t \right) \right\}}_{\text{Linear trend}} + \underbrace{\sum_{1 \leq i \leq \frac{\Delta t}{a/4}} \left\{ B_{\sin, i} \sin \left(\frac{2\pi i}{\Delta t} j(t) \right) + B_{\cos, i} \cos \left(\frac{2\pi i}{\Delta t} j(t) \right) \right\}}_{\text{Inter-annual variation}} + \underbrace{\sum_{1 \leq i \leq \frac{\Delta t}{a/4}} \left\{ C_{\sin, i} \sin \left(\frac{2\pi i}{\Delta t} k(t) \right) + C_{\cos, i} \cos \left(\frac{2\pi i}{\Delta t} k(t) \right) \right\}}_{\text{Intra-annual variation}}$$

Example of continuous time series of MUSICA IASI CH₄ and CH₄^{*} daily mean data retrieved in the surroundings of Tenerife Island between 2007 and 2017.



The yellow line is the a priori data used. The results of the multi-regression fit of the time series model are depicted as black line and the time series model components describing the long-term behavior are represented by the blue line.

The periods with different EUMETSAT L2 PPF software versions that can affect the MUSICA IASI products are indicated by magenta colour.

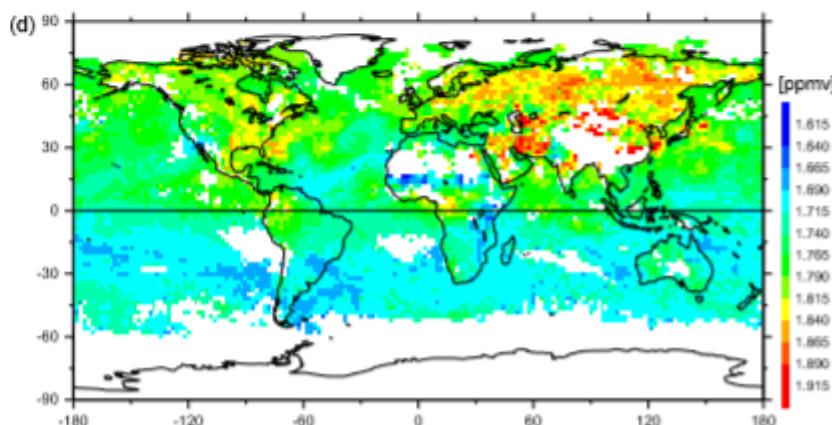
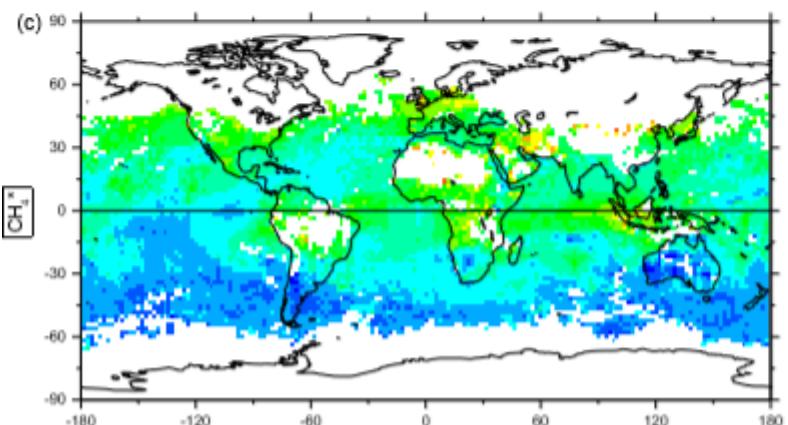
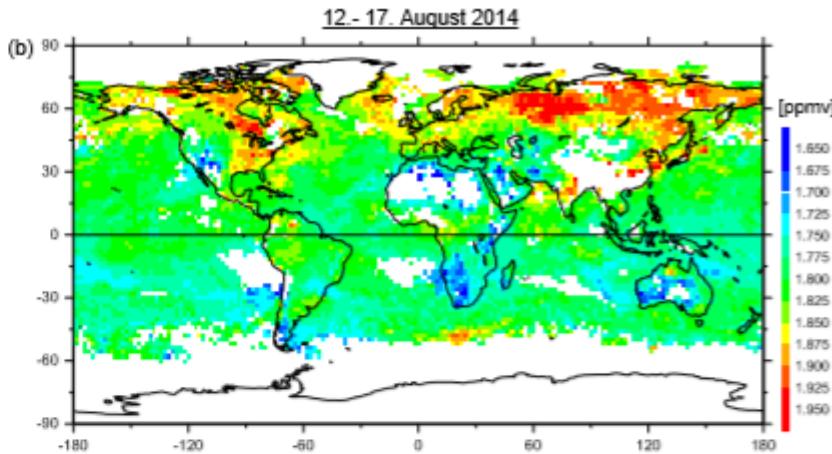
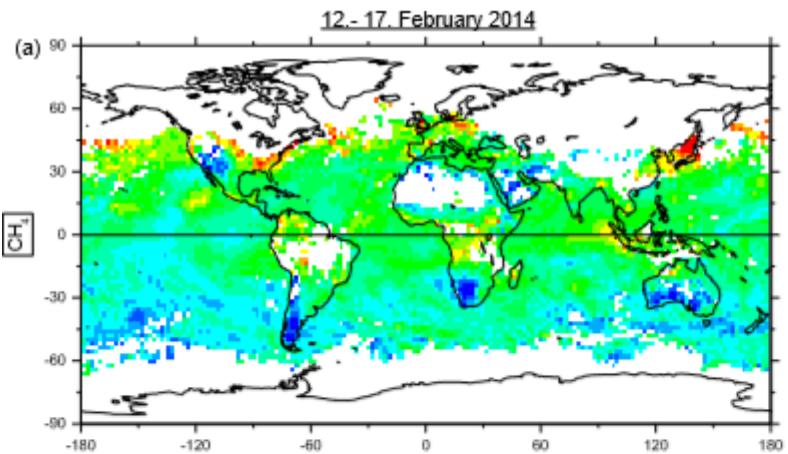
Time Series Model and Long-term Data Consistency

History of EUMETSAT Level 2 PPF software modification and EUMETSAT Level 2 data usage that can potentially affect the MUSICA IASI products.

Start date	PPF software	Relevance for MUSICA IASI product
27/11/2007	v4.0	Start of EUMETSAT operational Level 2 data dissemination.
14/09/2010	v5.0.6	Improvement of the EUMETSAT Level 2 middle/upper tropospheric temperatures (August et al., 2012), which are subsequently used as a priori by the MUSICA processor.
20/10/2011	v5.2.1	Change of the radiative transfer model used for EUMETSAT Level 2 cloud-free optimal estimation retrievals of atmospheric temperatures (EUMETSAT, 2017), which are subsequently used as a priori by the MUSICA processor.
30/09/2014	v6.0.5	Start using of EUMETSAT Level 2 land surface emissivities (instead of IREMIS, Seemann et al., 2008) for MUSICA processing over land. Change of pressure gridding used by the EUMETSAT Level 2 cloud-free optimal estimation retrievals of atmospheric temperatures (EUMETSAT, 2017), which are subsequently used as a priori by the MUSICA processor.

Geographical Coverage

Examples of global geographical distribution of the free tropospheric MUSICA IASI products retrieved at 4.2 km altitude, filtered for $c_{\text{sen}} < 50\%$ and averaged for an latitude x longitude area of $2^{\circ} \times 2^{\circ}$. (a) and (b) for CH_4 ; (c) and (d) for CH_4^* . The maps are shown separately for mid February 2014 (a and c) and mid August 2014 (b and d).



Geographical Coverage

Same as previous figure, but for the 10.9 km retrieval altitude.

