Ground-based remote sensing of tropospheric water vapour isotopologues at ten globally distributed NDACC sites

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Emmanuel Mahieu, Bernard Lejeune: Institute of Astrophysics and Geophysics, University of Liège, Belgium

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(1) The project MUSICA

(2) The contributing FTIR sites

(3) Charcterisation of the FTIR H2O and δD products: averaging kernels + error estimation

(4) Mid-infrared CO2 retrievals for documenting the network-wide data consistency

(5) Brief presentation of results

(6) Summary

(1) The project MUSICA

MUSICA: **MU**lti-plarform remote **S**ensing of **I**sotopologues for investigating the **C**ycle of **A**tmospheric water

Scientific Background: For understanding climate we have to understand the atmospheric water cycle (evapotration – transport – condenstaion - rainout), e.g.:

- Importance of latent heat budget
- processes that determine upper tropospheric H2O
- response of ice sheet retreat on atmospheric circulation

The ratio of water vapour isotopologues is very promising for investigating the water cycle: $\delta \mathrm{D} = 1000‰ \times \left(\frac{[\mathrm{HD}^{16}\mathrm{O}]/[\mathrm{H}_2^{16}\mathrm{O}]}{\mathrm{SMOW}} - 1\right)$

BUT: So far there is a lack of observational data with a documented high quality.

Objective of MUSICA: MUSICA provides a unique global long-term atmospheric water vapour isotopologue dataset of a **high and well documented quality.** It is mainly a data producing project. The scientific interpretation will be made in collaboration with the modeling community.

(1) The project MUSICA

Strategy of MUSICA: Combine different measurement techniques:

(1) Ground-based NDACC FTIR observations: high quality data, continuous observation, long-term time series

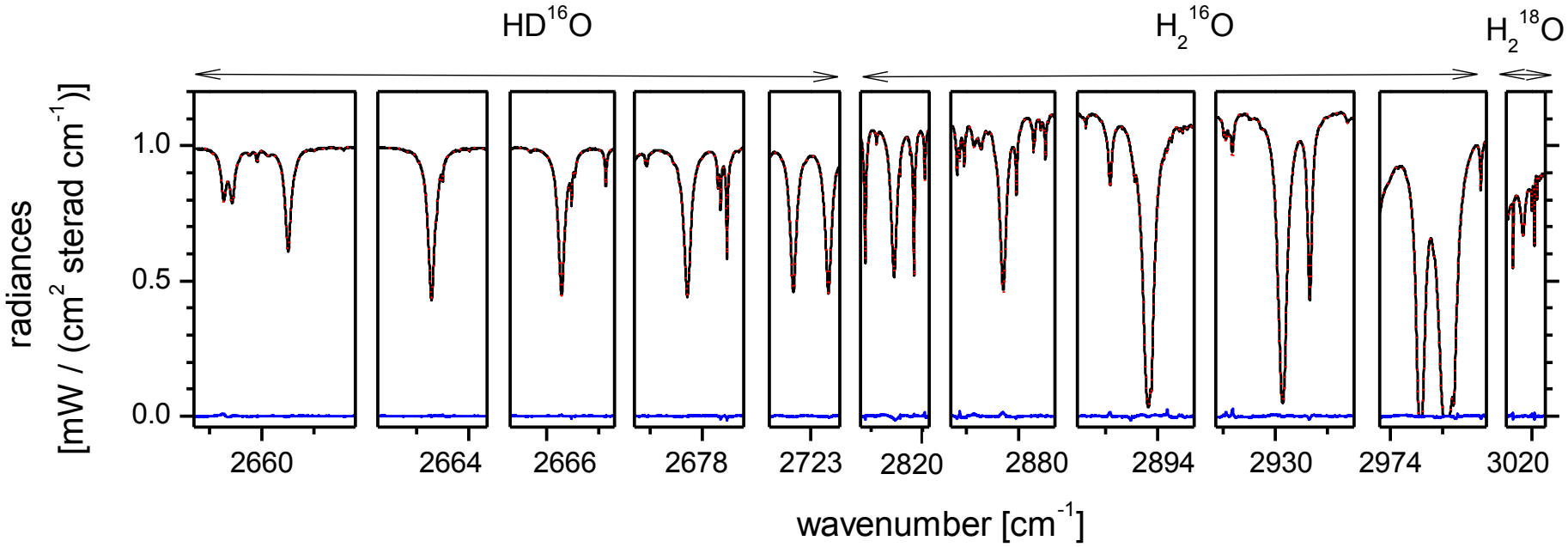
(2) Space-based IASI/Metop observations: global coverage twice per day, long-term funding assured, high resolution mid-infrared spectra

(3) In-situ measurements: direct calibration wrt standards, can serve as refernce measurements for the remote sensing observations

Acknowledgement: The project MUSICA is funded by the European Research Council under the European Community's Seventh Framework Programme (FP7/2007-2013) / ERC Grant agreement n° 256961.

(3) Characterisation of the ground-based FTIR products

The applied spectral microwindows:



-!strong, but not saturated, and well isolated HDO signatures

-!strong, but not saturated, and well isolated H2O signatures

→ we expect optimal sensitivity and precision for isotopologue retrievals

MUSICA ‘s optimal estimation inversion procedure

The MUSICA inversion precedure uses a priori knowledge of H2O and HDO and in addition of HDO/H2O.

Method: transfer the atmospheric states, Jacobians, and a priori covariances on a logarithmic scale and expand the a priori matrix $\mathbf{S_a}$:

$$[\vec{y} - \vec{f}(\vec{x}, \vec{b}, \vec{p})]^T \mathbf{S_\epsilon}^{-1} [\vec{y} - \vec{f}(\vec{x}, \vec{b}, \vec{p})] + [\vec{x} - \vec{x_a}]^T \mathbf{S_a}^{-1} [\vec{x} - \vec{x_a}]$$

$$\mathbf{S_a} = \begin{pmatrix} \mathbf{S_{aH}} + \frac{1}{2}\mathbf{S_{aI}} & \mathbf{S_{aH}} - \frac{1}{2}\mathbf{S_{aI}} \\ \mathbf{S_{aH}} - \frac{1}{2}\mathbf{S_{aI}} & \mathbf{S_{aH}} + \frac{1}{2}\mathbf{S_{aI}} \end{pmatrix}$$

Our retrieval considers the a priori cross covariance between H_2O and HDO: we constrain ln[HDO]-ln[H_2O].

$\mathbf{S_a}$ has large outer diagonal elements!

The proper description of the water isotopologue state

H2O and HDO vary largly in parallel (are strongly correlated), the ratio HDO/H2O (or δD) varies much less.

The actual atmospheric water vapour state is much better discribed by the two state vectors **(ln[H2O] + ln[HDO])/2** and **(ln[HDO] - ln [H2O])**.

Our inversion precedure performs an optimal estimation of these states. This becomes visible by a basis transformation:

$$\mathbf{S}'_\mathbf{a} = \mathbf{P}^T \mathbf{S}_\mathbf{a} \mathbf{P}$$

$$= \begin{pmatrix} \frac{1}{2}\mathbb{I} & -\mathbb{I} \\ \frac{1}{2}\mathbb{I} & \mathbb{I} \end{pmatrix}^T \begin{pmatrix} \mathbf{S_{aH}} + \frac{1}{2}\mathbf{S_{aI}} & \mathbf{S_{aH}} - \frac{1}{2}\mathbf{S_{aI}} \\ \mathbf{S_{aH}} - \frac{1}{2}\mathbf{S_{aI}} & \mathbf{S_{aH}} + \frac{1}{2}\mathbf{S_{aI}} \end{pmatrix} \begin{pmatrix} \frac{1}{2}\mathbb{I} & -\mathbb{I} \\ \frac{1}{2}\mathbb{I} & \mathbb{I} \end{pmatrix}$$

$$= \begin{pmatrix} \mathbf{S_{aH}} & 0 \\ 0 & \mathbf{S_{aI}} \end{pmatrix}$$

The columns of **P** are the new basis vectors: **(ln[H2O] + ln[HDO])/2** and **(ln [HDO] - ln[H2O])**.

This basis vectors are a good proxies for the H2O and δD

1: (ln[H2O] + ln[HDO])/2, a proxy for the H2O state

$$\Delta\left(\frac{\ln[\mathrm{H_2O}]+\ln[\mathrm{HDO}]}{2}\right) \approx \frac{\Delta(\sqrt{[\mathrm{H_2O}][\mathrm{HDO}]})}{\sqrt{[\mathrm{H_2O}][\mathrm{HDO}]}} \approx \frac{\Delta[\mathrm{H_2O}]}{[\mathrm{H_2O}]}$$

Changes in (ln[H2O] + ln[HDO])/2 are well representative for relative changes in H2O:

2: (ln[HDO] - ln[H2O]), a proxy for the δD state

$$\Delta(\ln[\mathrm{HDO}]-\ln[\mathrm{H_2O}]) \approx \frac{\Delta\left(\frac{[\mathrm{HDO}]}{[\mathrm{H_2O}]}\right)}{\frac{[\mathrm{HDO}]}{[\mathrm{H_2O}]}} \approx \frac{\Delta\left(\frac{[\mathrm{HDO}]}{[\mathrm{H_2O}]}\right)}{\mathrm{SMOW}} = \Delta(\delta\mathrm{D})$$

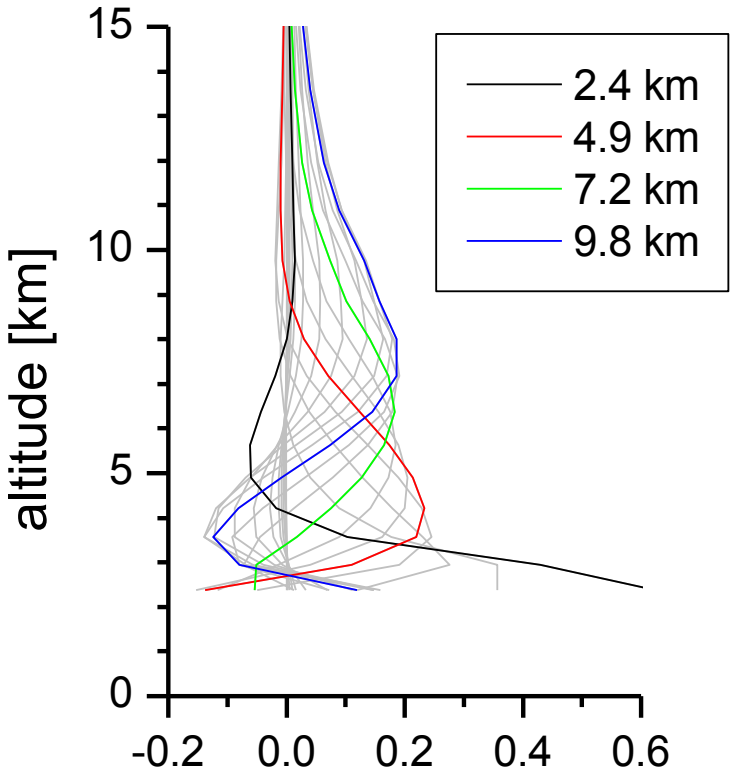
Changes in (ln[HDO] - ln[H2O]) are well representative for changes in δD:

→ Our inversion procedure performs in deed an optimal estimation of H2O and δD!

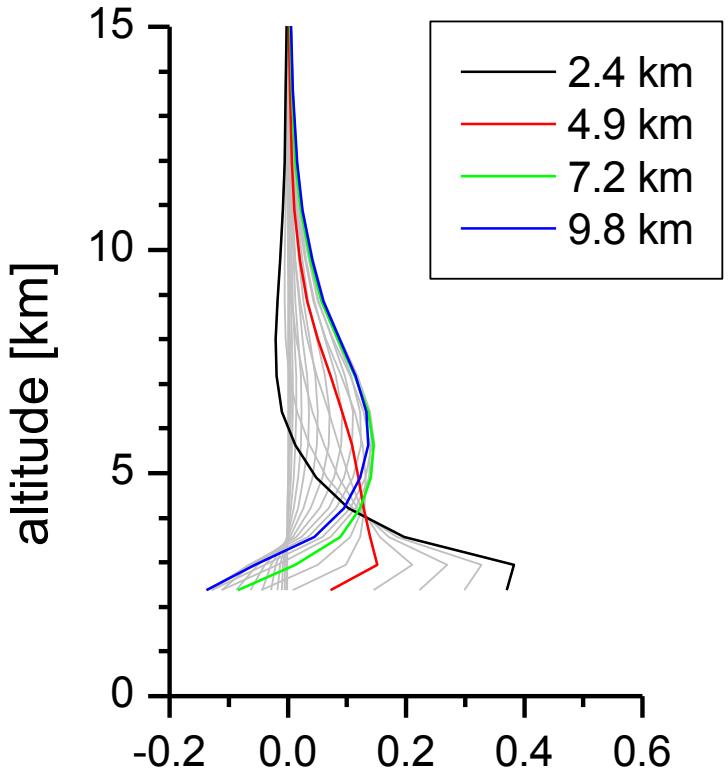
→ In the proper orthogonal basis we can well characterise the retrieved H2O and δD products

Averaging kernels

OE of H_2O



OE of isotopology



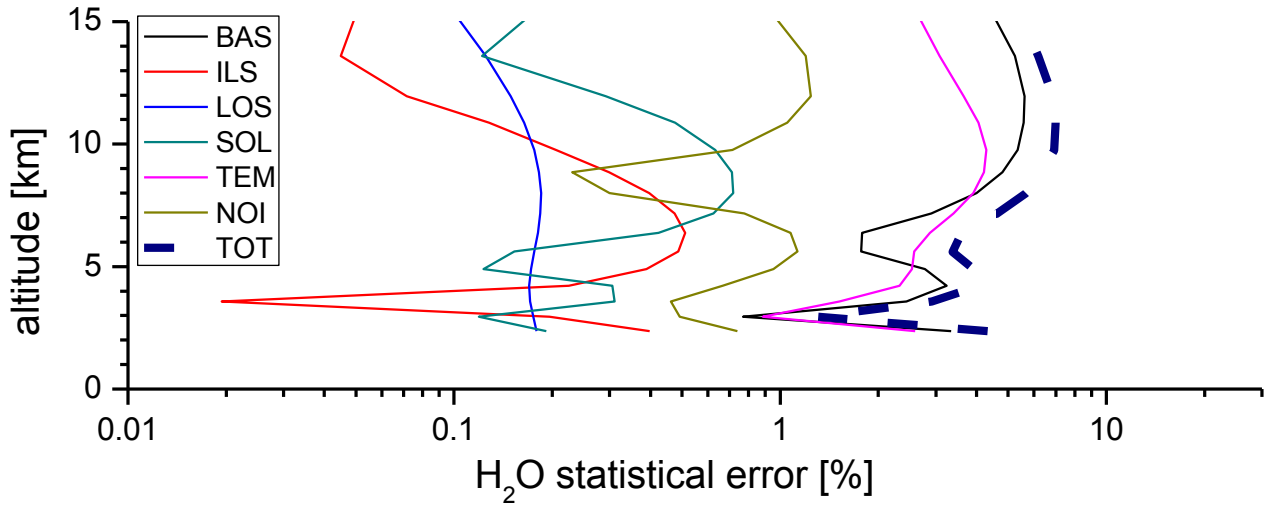
MUSICA provides two data products:

(1)!Optimal estimation of the H2O state (DOF: 2.9)

(2)!Optimal estimation of water vapour isotopology state (DOF: 1.7)

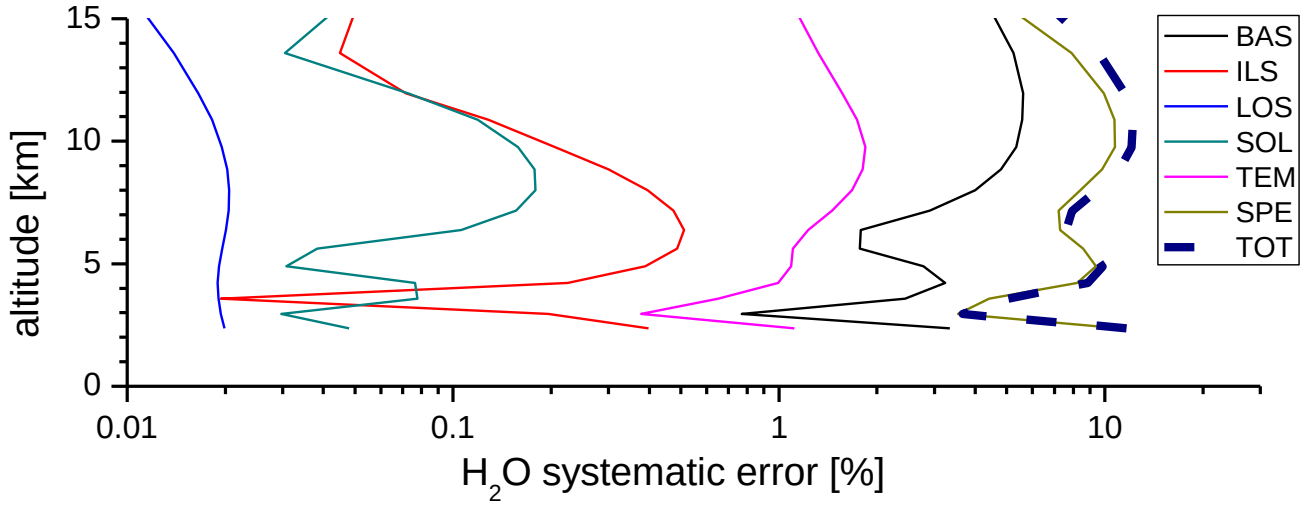
(4) Error estimation

Statistical errors for an OE retrieval of the H_2O state:



Leading error sources: measurement noise, temperature profile and baseline

Systematic errors for an OE retrieval of the H_2O state:



Leading error sources: baseline and spectroscopic parameters

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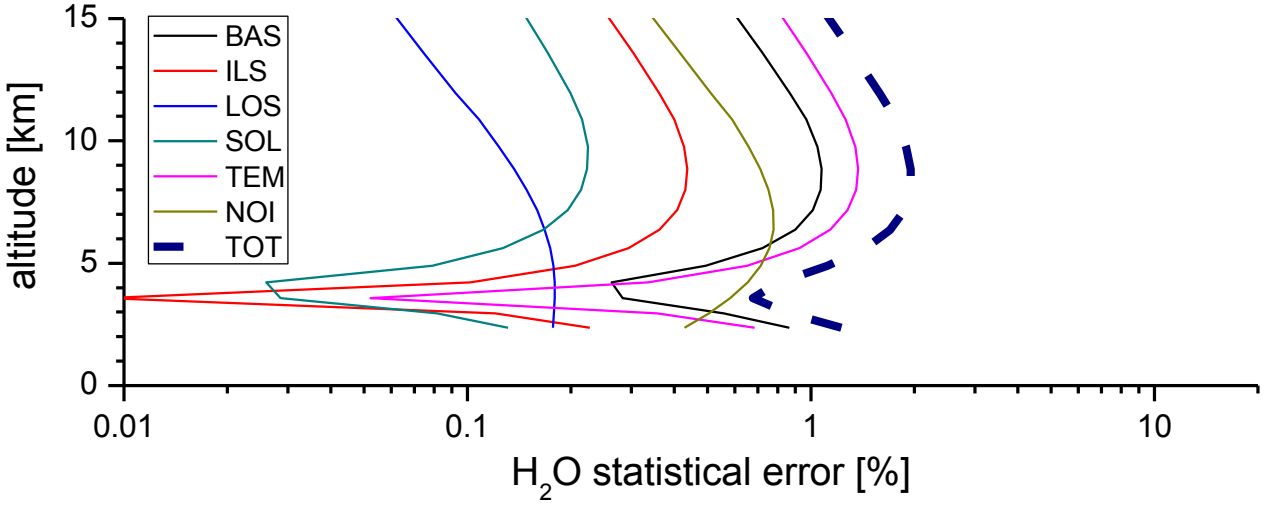
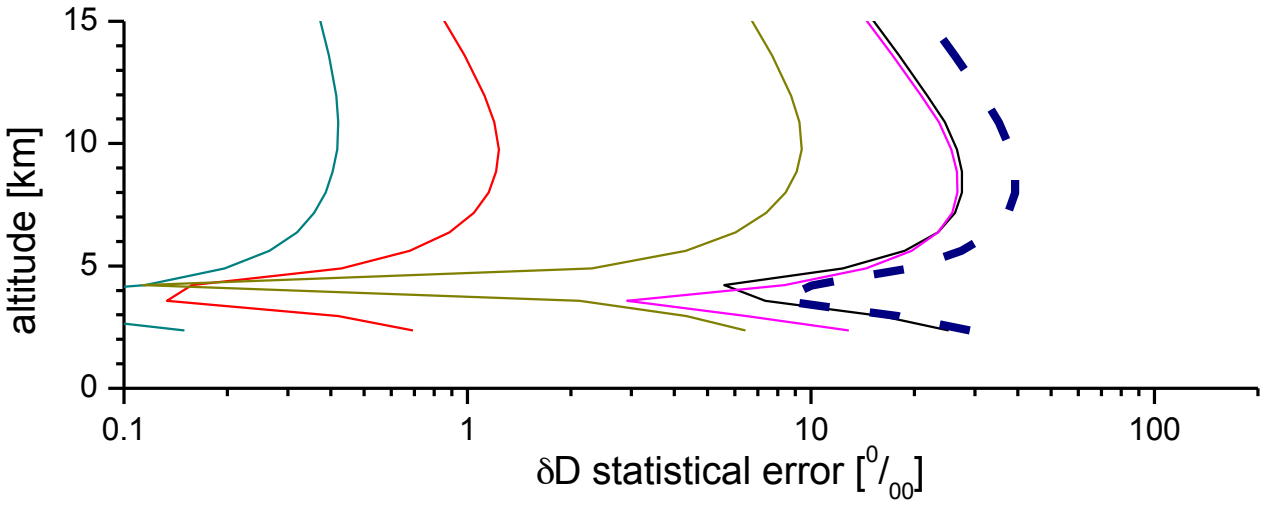
Total column errors for an OE of the H_2O state:

Error (acronym)	Statistical	Systematical
NOI	0.6%	–
BAS	0.4%	0.4%
ILS	<0.1%	<0.1%
TEM	0.2%	0.1%
LOS	0.2%	<0.1%
SOL	<0.1%	<0.1%
SPE	–	1.0%
Total (TOT)	0.8%	1.1%
Smoothing error	0.1%	–

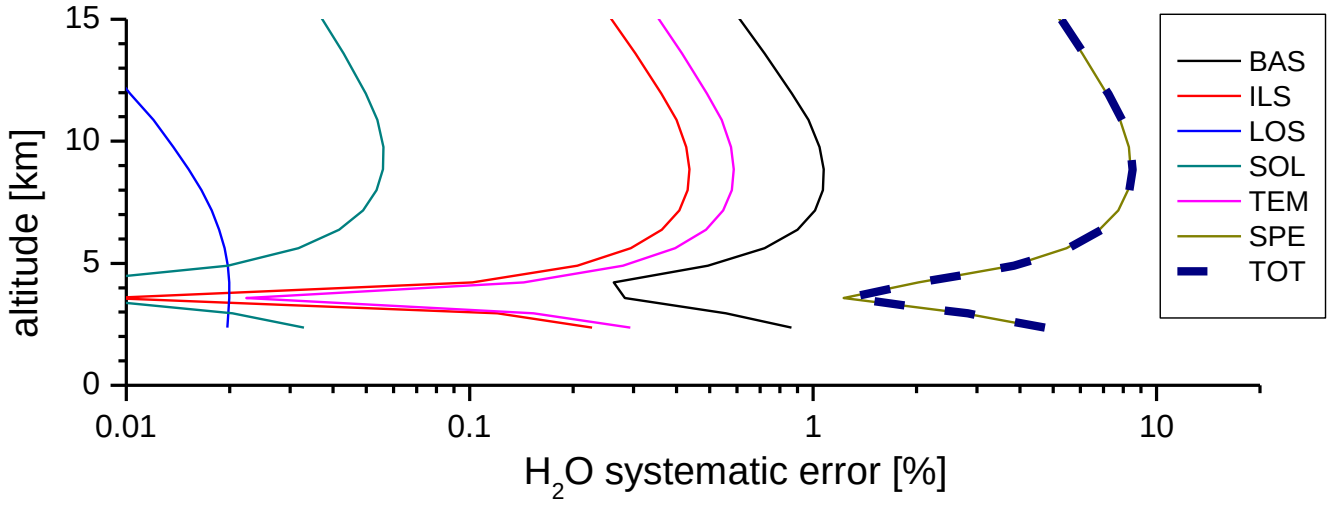
Statistical errors for an OE retrieval of the isotopology state (after applying the a posteriori operator):

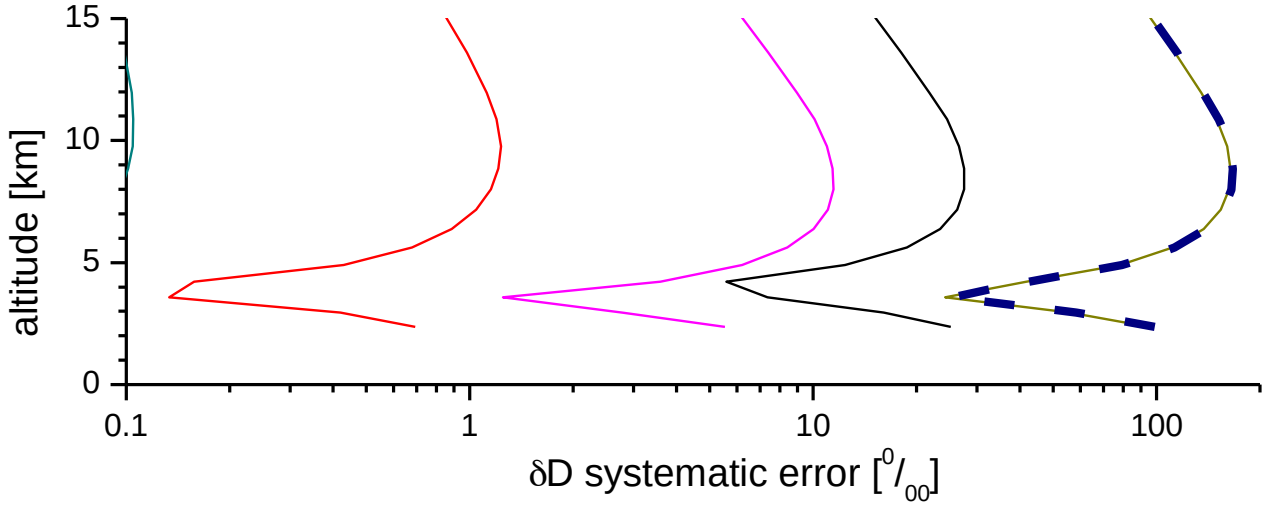




Leading error sources: measurement noise, baseline, and temperature profile

Systematic errors for an OE retrieval of the isotopology state (after applying the a posteriori operator):





Leading error source: spectroscopic parameters

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Total column errors for an OE of the isotopology state (after applying the a posteriori operator):

H2O

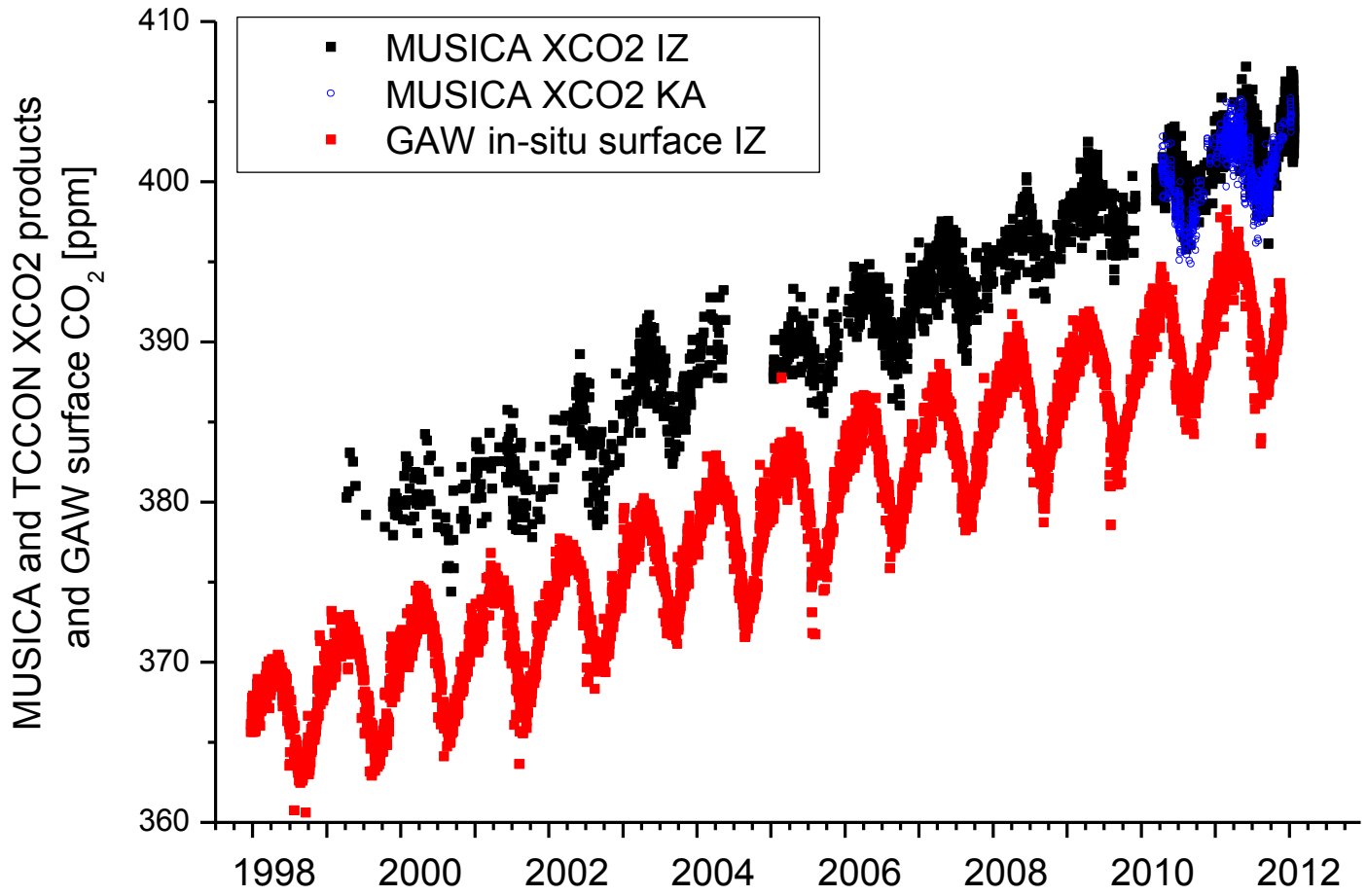
Error (acronym)	Statistical	Systematical
NOI	0.6%	–
BAS	0.2%	0.2%
ILS	<0.1%	<0.1%
TEM	0.1%	<0.1%
LOS	0.2%	<0.1%
SOL	<0.1%	<0.1%
SPE	–	1.1%
Total (TOT)	0.7%	1.2%
Smoothing error	2.5%	–

δD

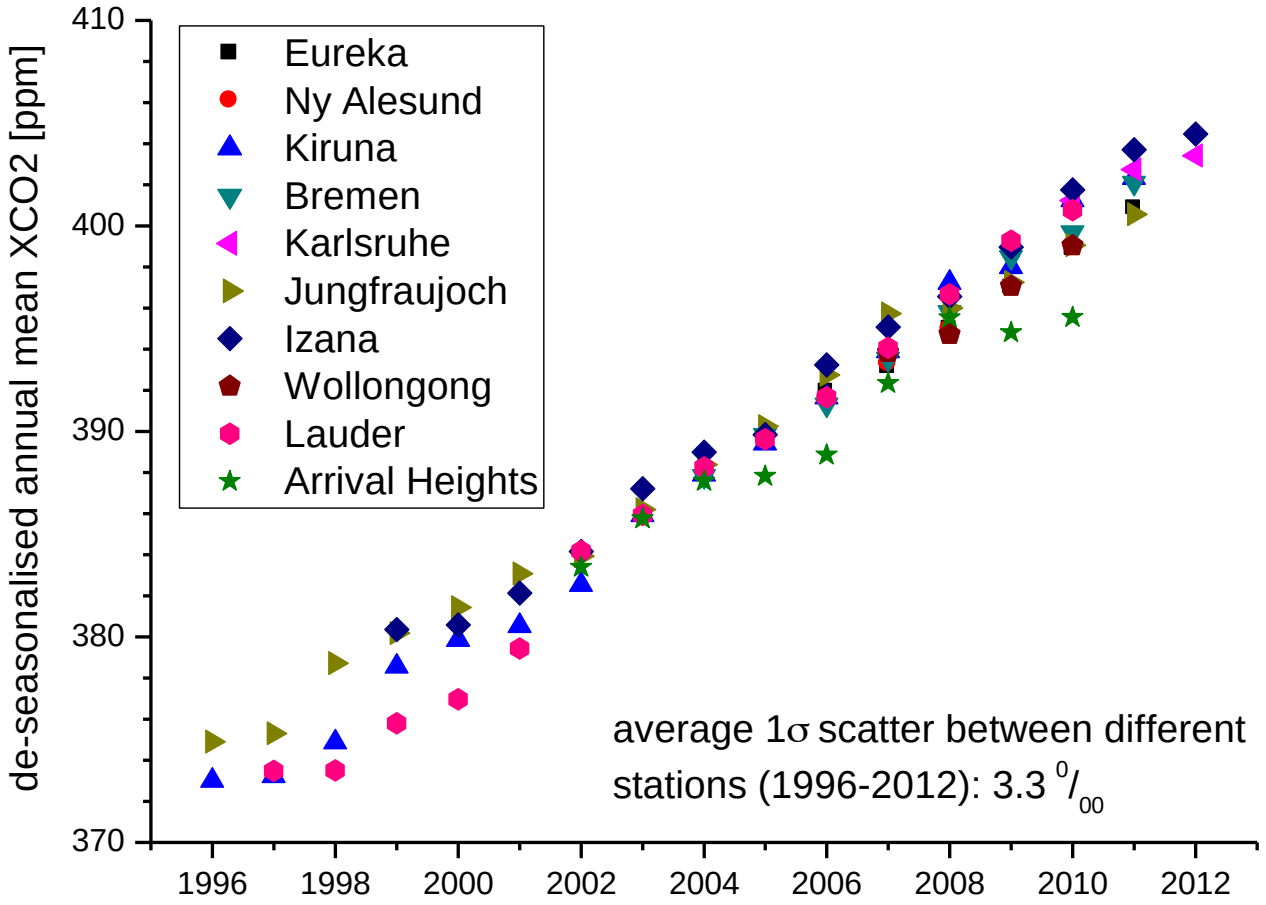
Error (acronym)	Statistical	Systematical
NOI	1.4‰	–
BAS	5.9‰	5.9‰
ILS	<0.1‰	<0.1‰
TEM	3.2‰	1.2‰
LOS	<0.1‰	<0.1‰
SOL	<0.1‰	<0.1‰
SPE	–	22.4‰
Total (TOT)	6.9‰	23.3‰
H_2O interference error	0.3‰	–
Smoothing error	2.0‰	–

(4) Network-wide consistency (documented by the MUSICA mid-infrared CO2 product, 2620 - 2630cm^{-1})

MUSICA CO_2 time series, example Izaña and Karlsruhe:

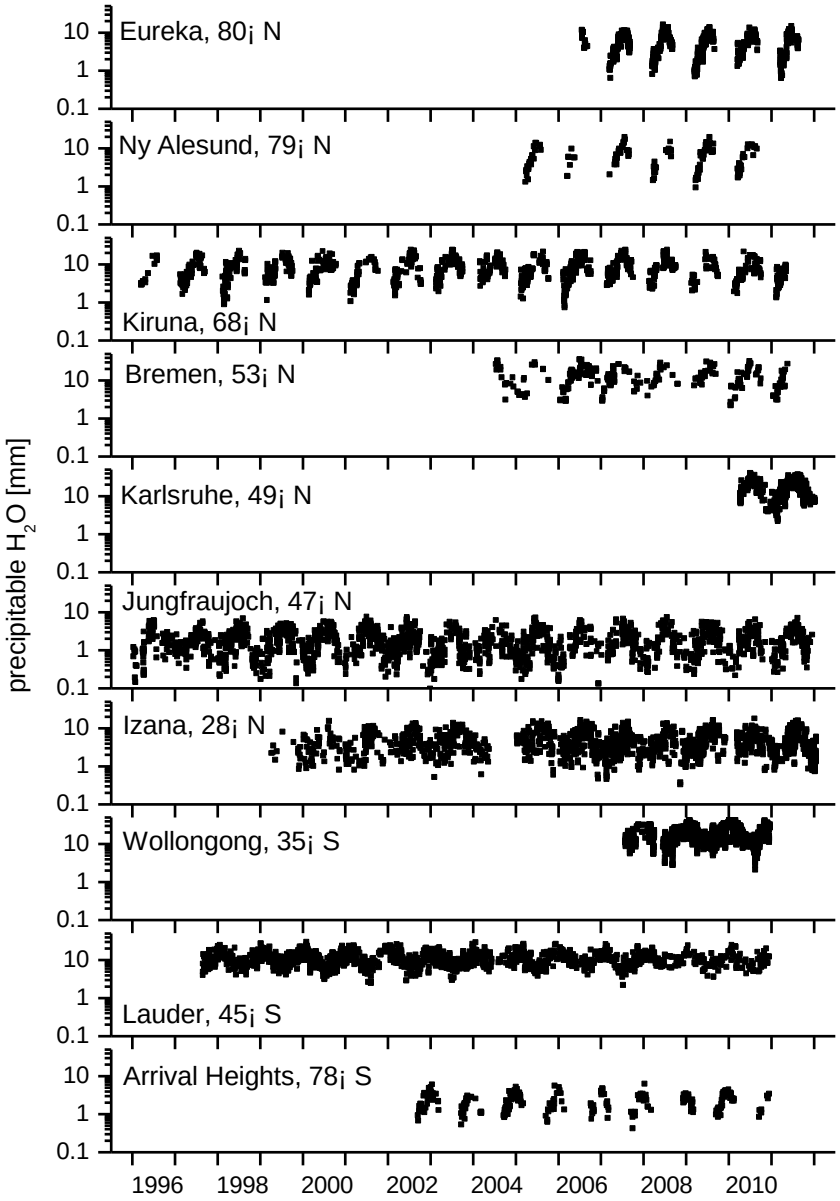


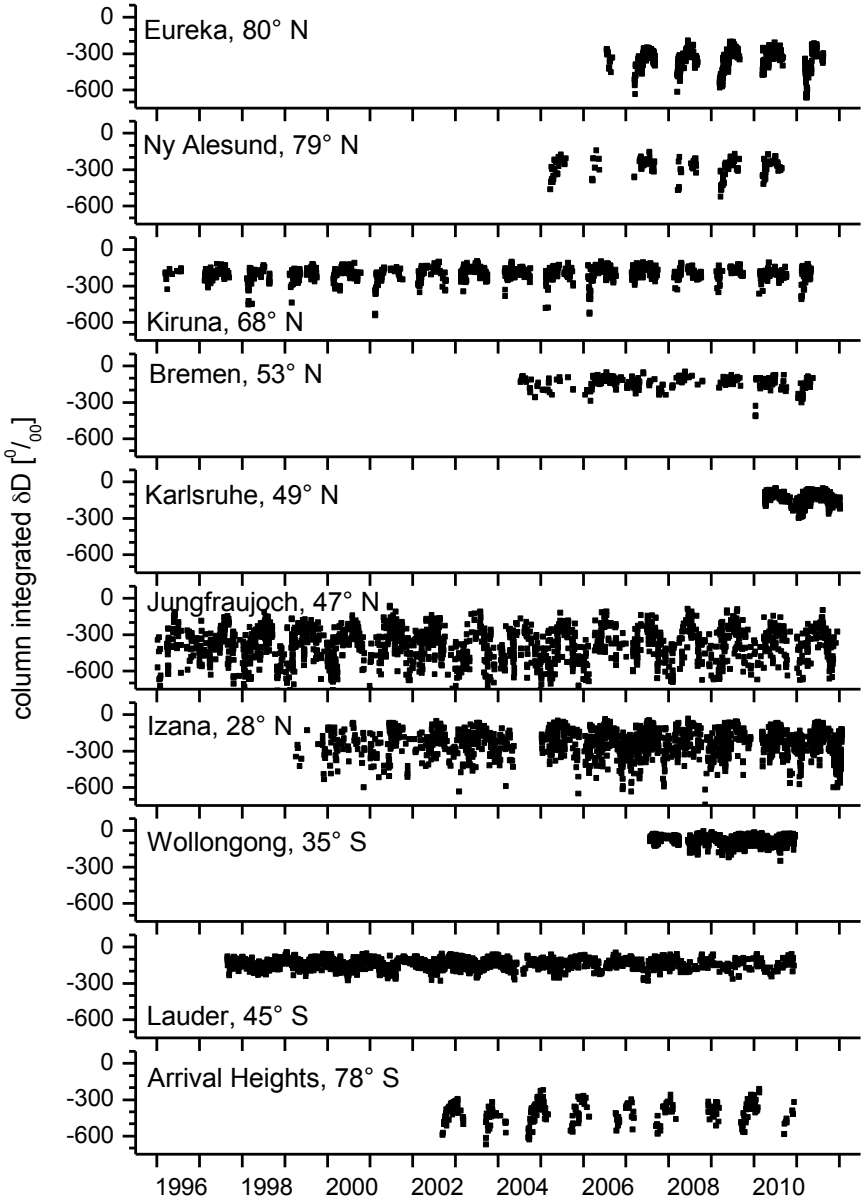
De-seasonalised annual mean XCO2 obtained from mid-infrared spectra (2620 - 2630cm^{-1}) at all MUSICA stations



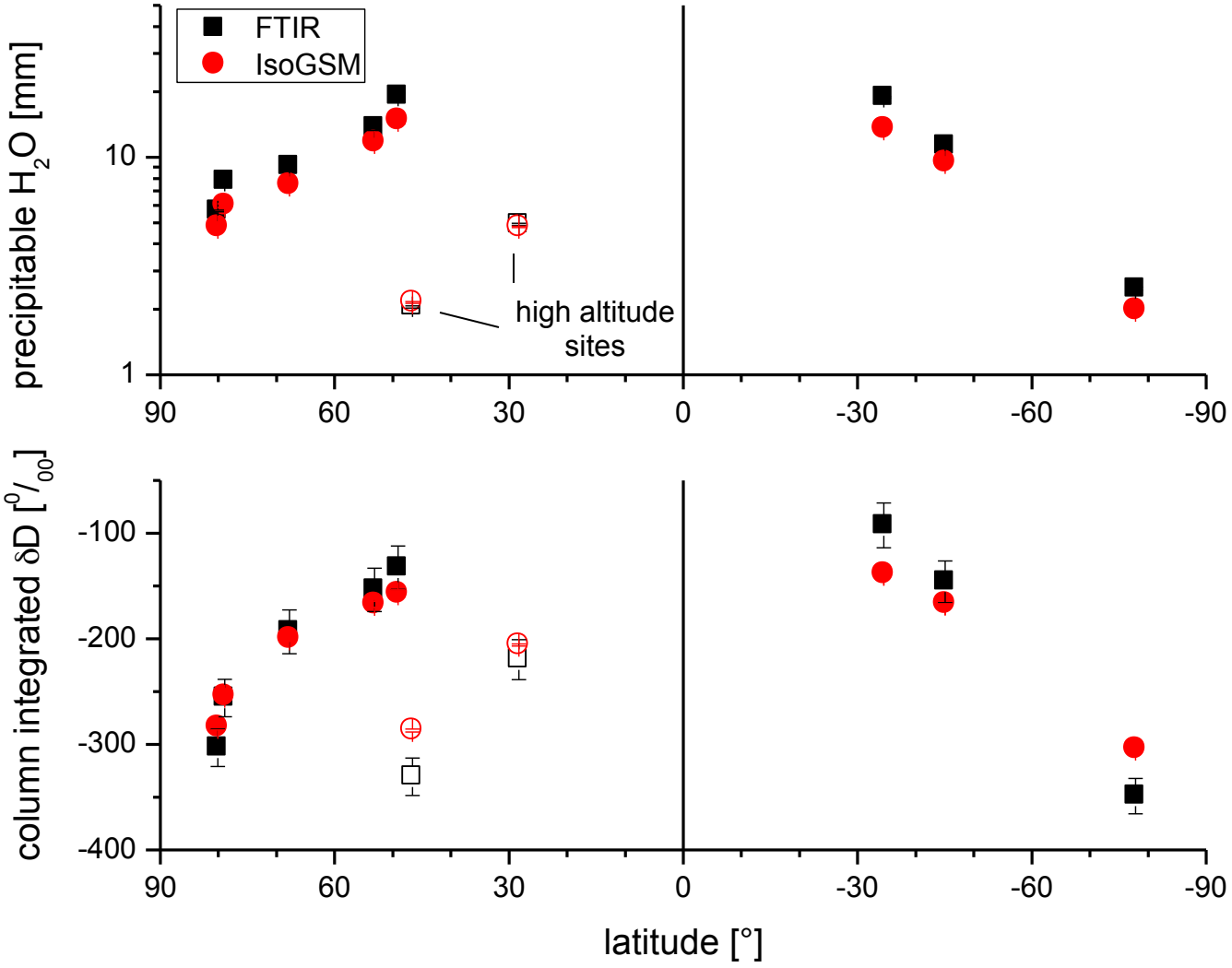
This nicely documents the good work done by the many PhD students, PostDocs, Scientists, Technicians, etc., involved in the FTIR measurements!

(5) Brief presentation of results (dataset (1996 -2012)





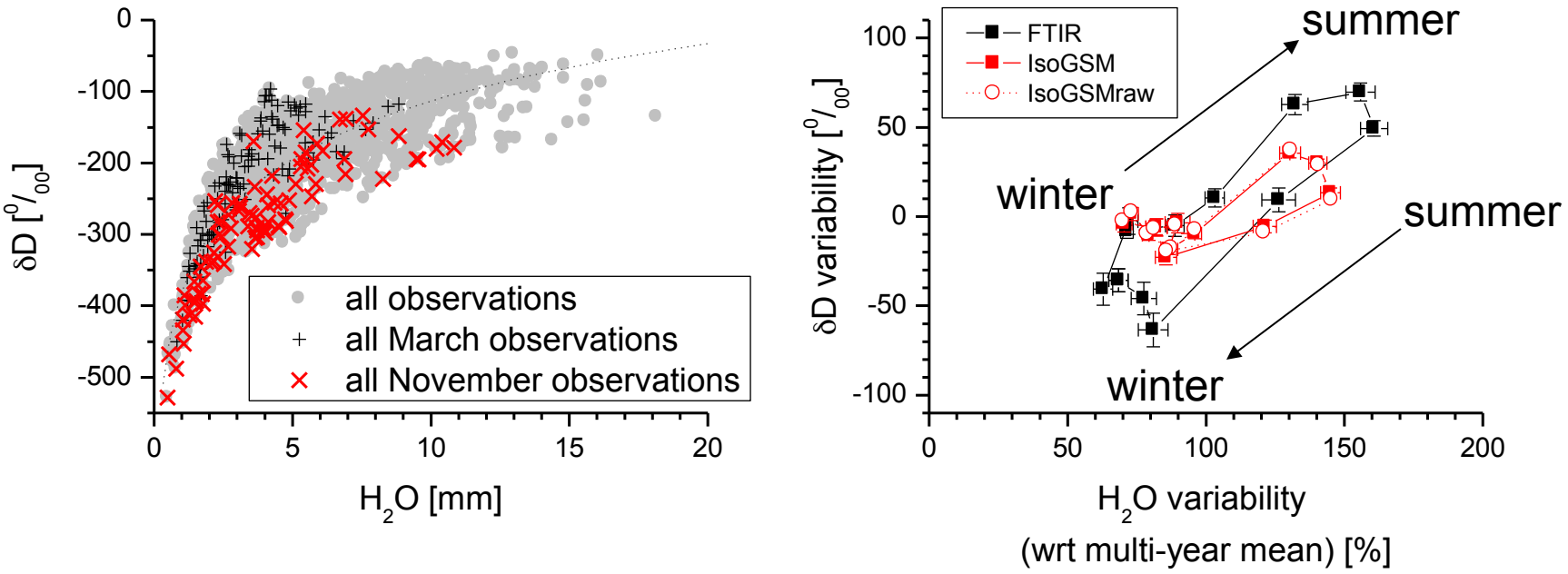
Multi-year means (overview all sites)



Model IsoGSM: Yoshimura et al., JGR, 2008.

Multi-year annual cycles (H2O-δD plots):

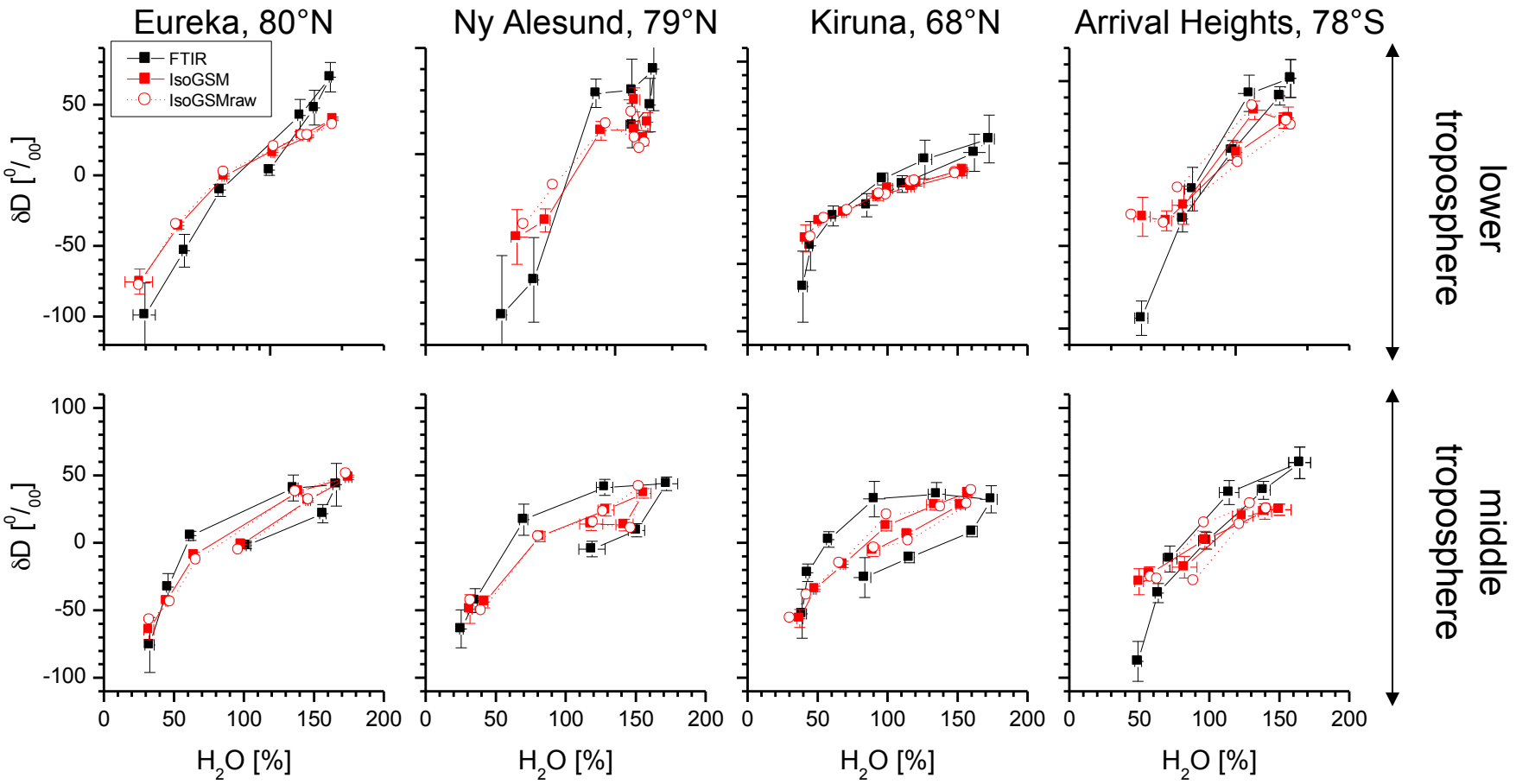
Example Izaña:



FTIR: Passing from summer to winter, the troposphere is more depleted in heavy isotopologues than passing from winter to summer (→ spring and autumn humidity „is not the same“)

Model IsoGSM: This detail in the observed annual tropospheric water cycle is, although indicated, not fully captured by the model IsoGSM.

Annual cycles, example polar sites



The differences between the summer-to-winter and winter-to-summer transitions are mostly present in the middle troposphere! This tendency is also indicated in the model IsoGSM. The agreement between FTIR and IsoGSM is better in the lower than in the middle troposphere.

(6) Summary

- The MUSICA project provides two ground-based FTIR water vapour products:
  (1) OE of H2O (degree of freedom of ≈3; sensitive up to upper troposphere).
  (2) OE of isotopology (degree of freedom of 1.5-2; sensitive up to middle tropopshere).

- Estimated precision for OE of H2O: <5% (total columns: <1%)

-!Estimated precision for OE of isotopology: H2O profiles <2%; δD profiles <30‰

-!Error bars are provided for each individual observation!

-!The MUSICA CO_2 retrievals document a good network-wide data consistency.

→ The high potential of the gb FTIR network has been demonstated

Next step (1): discuss with the collaborating FTIR groups the details of the planned MUSICA database.

Next step (2): discuss the participation in GRUAN (J. Hannigan and M. Schneider are members of the GRUAN TT5: „Auxiliary Measurement Techniques“)

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EXTRA SLIDES

(2) Retrieval background

Innovation: using a priori knowledge of H2O (and HDO) and in addition of HDO/H2O.

Method: transfering the atmospheric states, Jacobians, and a priori covariances on a logarithmic scale and expand the a priori matrix $\mathbf{S_a}$:

$$[\vec{y} - \vec{f}(\vec{x}, \vec{b}, \vec{p})]^T \mathbf{S_\epsilon}^{-1} [\vec{y} - \vec{f}(\vec{x}, \vec{b}, \vec{p})] + [\vec{x} - \vec{x_a}]^T \mathbf{S_a}^{-1} [\vec{x} - \vec{x_a}]$$

$$\begin{pmatrix} \mathbf{S}^{-1}_{a,H_2O} & 0\ 0\ 0 \\ & 0\ 0\ 0 \\ & 0\ 0\ 0 \\ 0\ 0\ 0 & \\ 0\ 0\ 0 & \mathbf{S}^{-1}_{a,\mathrm{HDO}} \\ 0\ 0\ 0 & \end{pmatrix} + \left\{ \begin{pmatrix} \frac{1}{c_1} & 0 & 0 & -\frac{1}{c_1} & 0 & 0 \\ 0 & \frac{1}{c_2} & 0 & 0 & -\frac{1}{c_2} & 0 \\ 0 & 0 & \frac{1}{c_3} & 0 & 0 & -\frac{1}{c_3} \\ -\frac{1}{c_1} & 0 & 0 & \frac{1}{c_1} & 0 & 0 \\ 0 & -\frac{1}{c_2} & 0 & 0 & \frac{1}{c_2} & 0 \\ 0 & 0 & -\frac{1}{c_3} & 0 & 0 & \frac{1}{c_3} \end{pmatrix} + \begin{pmatrix} \frac{1}{a_1} & -\frac{1}{a_1} & 0 & -\frac{1}{a_1} & \frac{1}{a_1} & 0 \\ -\frac{1}{a_1} & (\frac{1}{a_1}+\frac{1}{a_2}) & -\frac{1}{a_2} & \frac{1}{a_1} & -(\frac{1}{a_1}+\frac{1}{a_2}) & \frac{1}{a_2} \\ 0 & -\frac{1}{a_2} & \frac{1}{a_2} & 0 & \frac{1}{a_2} & -\frac{1}{a_2} \\ -\frac{1}{a_1} & \frac{1}{a_1} & 0 & \frac{1}{a_1} & -\frac{1}{a_1} & 0 \\ \frac{1}{a_1} & -(\frac{1}{a_1}+\frac{1}{a_2}) & \frac{1}{a_2} & -\frac{1}{a_1} & (\frac{1}{a_1}+\frac{1}{a_2}) & -\frac{1}{a_2} \\ 0 & \frac{1}{a_2} & -\frac{1}{a_2} & 0 & -\frac{1}{a_2} & \frac{1}{a_2} \end{pmatrix} \right\}$$

Independent OE of H_2O and HDO

OE of HDO/H_2O

Schneider et al., Atmos. Chem. Phys., 6, 4705-4722, 2006.

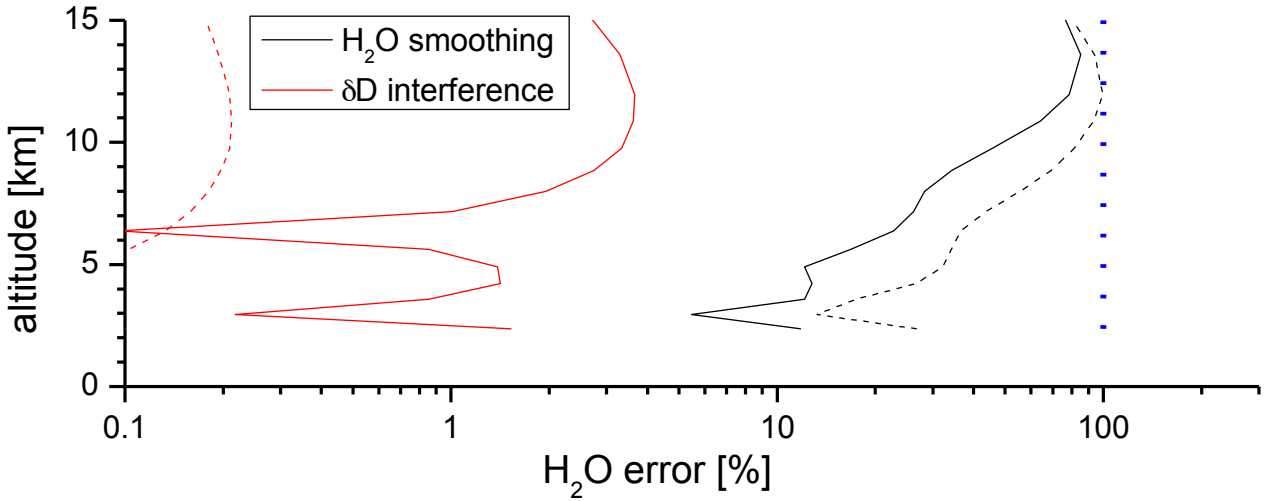
The „two step“ retrieval (a posteriori operator)

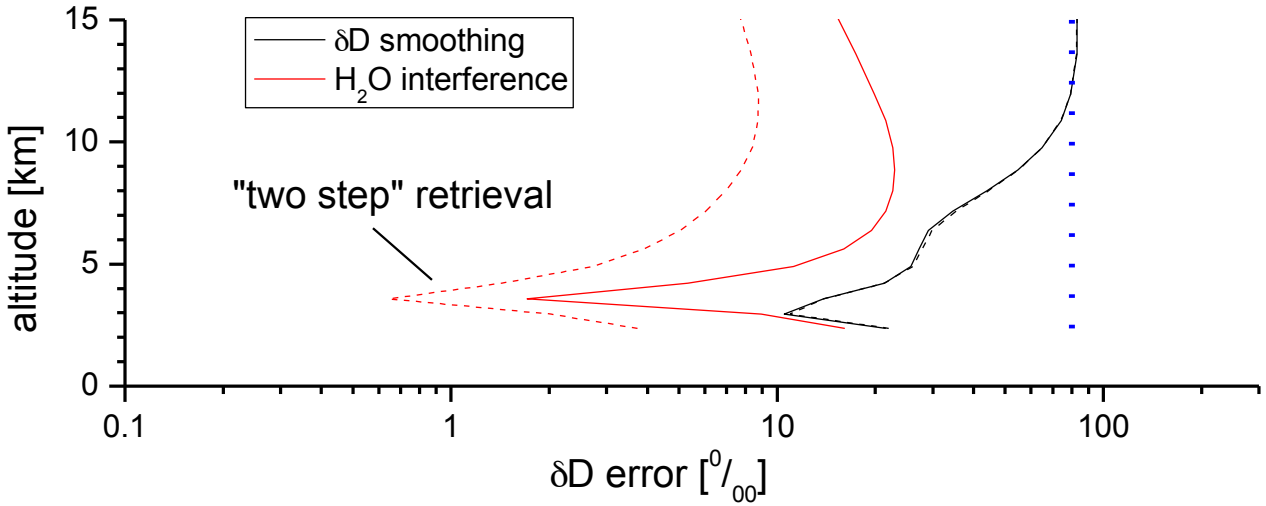
A posteriori operator **C**: $\mathbf{C} = \begin{pmatrix} \mathbf{A'_{II}} & 0 \\ -\mathbf{A'_{HI}} & \mathbb{I} \end{pmatrix}$

Effect of the a posteriroi operator on the averaging kernels:

$$
\begin{aligned}
\mathbf{A''} &= \mathbf{C}\mathbf{A'} \\
&= \begin{pmatrix} \mathbf{A'_{II}} & 0 \\ -\mathbf{A'_{HI}} & \mathbb{I} \end{pmatrix} \begin{pmatrix} \mathbf{A'_{HH}} & \mathbf{A'_{IH}} \\ \mathbf{A'_{HI}} & \mathbf{A'_{II}} \end{pmatrix} \\
&= \begin{pmatrix} \mathbf{A'_{II}}\mathbf{A'_{HH}} & \mathbf{A'_{II}}\mathbf{A'_{IH}} \\ -\mathbf{A'_{HI}}\mathbf{A'_{HH}} + \mathbf{A'_{HI}} & -\mathbf{A'_{HI}}\mathbf{A'_{IH}} + \mathbf{A'_{II}} \end{pmatrix} \\
&= \begin{pmatrix} \mathbf{A''_{HH}} & \mathbf{A''_{IH}} \\ \mathbf{A''_{HI}} & \mathbf{A''_{II}} \end{pmatrix}
\end{aligned}
$$

Smoothing error and intereference error



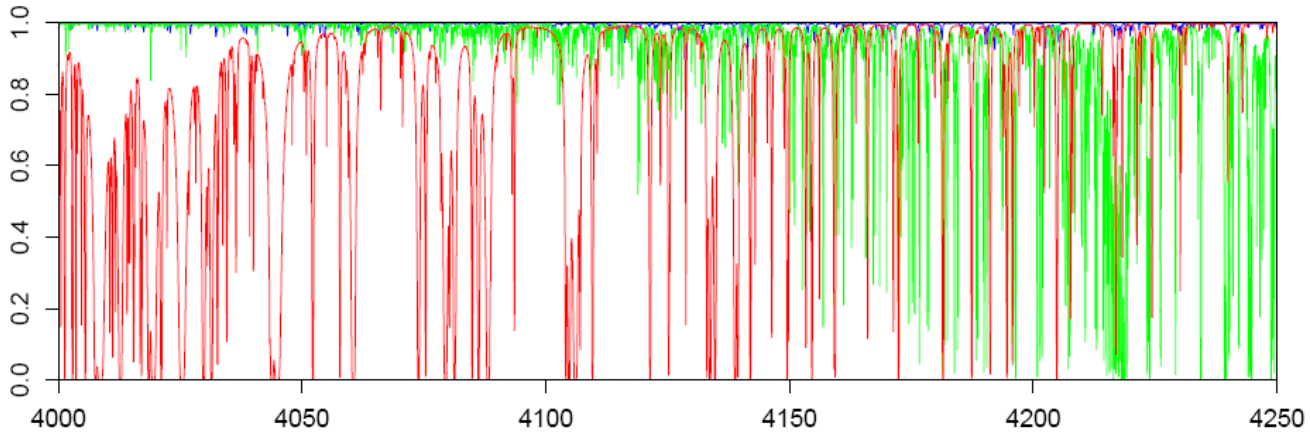


The „two step“ retrieval significantly reduces the interference of humidity on δD!

Outlook: NDACC and TCCON δD retrievals?

For TCCON δD products there is so far no similar quality documentation!

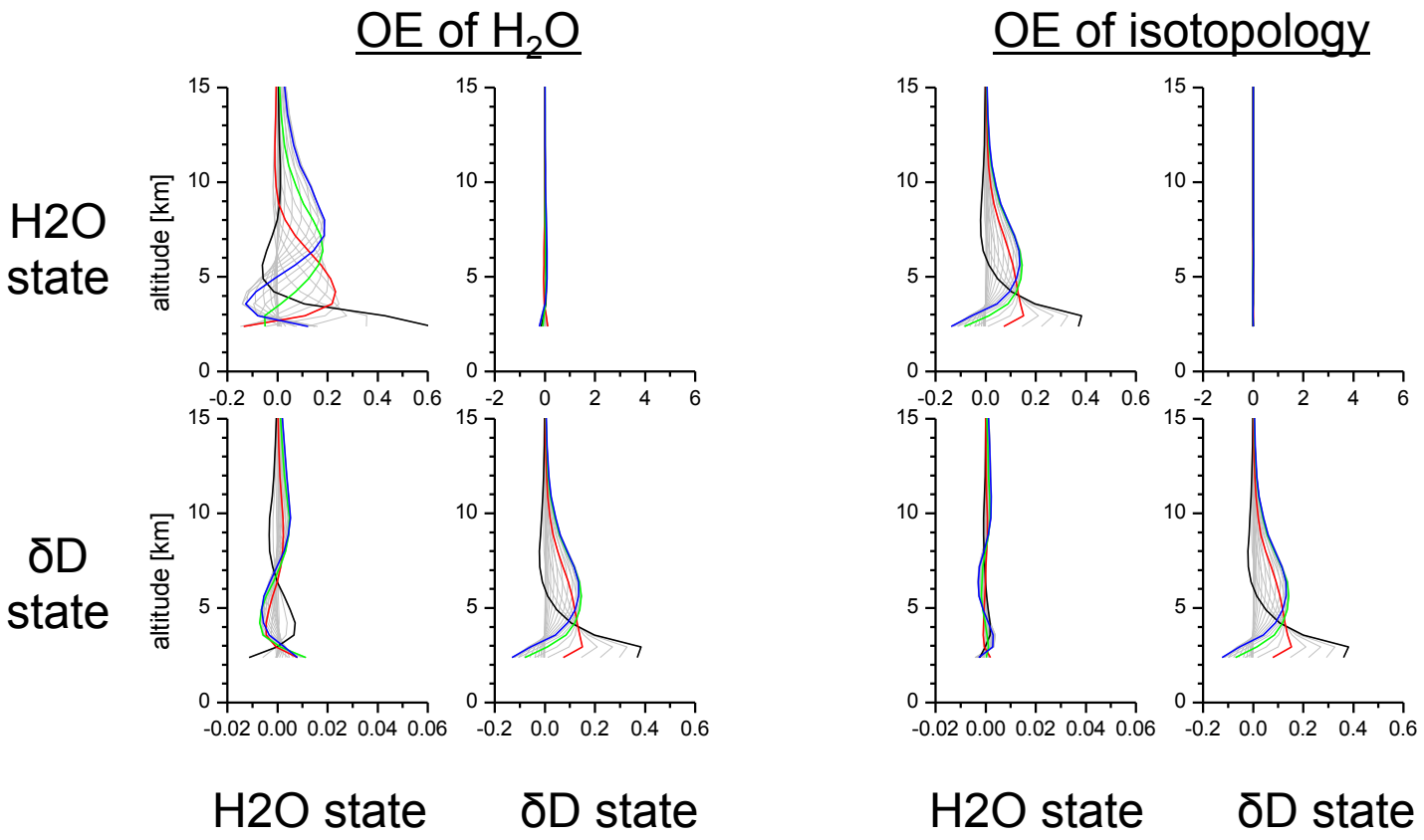
TCCON spectra cover the near infrared (>3800 cm^{-1}). Near infrared region with strongest $HD^{16}O$ absorption signatures (4000 – 4250 cm^{-1}):



→ the TCCON $HD^{16}O$ signature is very weak and TCCON δD data might be significantly affected by the actual H_2O and CH_4 amounts.

→ Further studies are needed!

Kernels ({(ln[H2O]+ln[HDO])/2, (ln[HDO]-ln[H2O])}-basis)



MUSICA provides two data products:

(1)!Optimal estimation of the H2O state (DOF: 2.9)

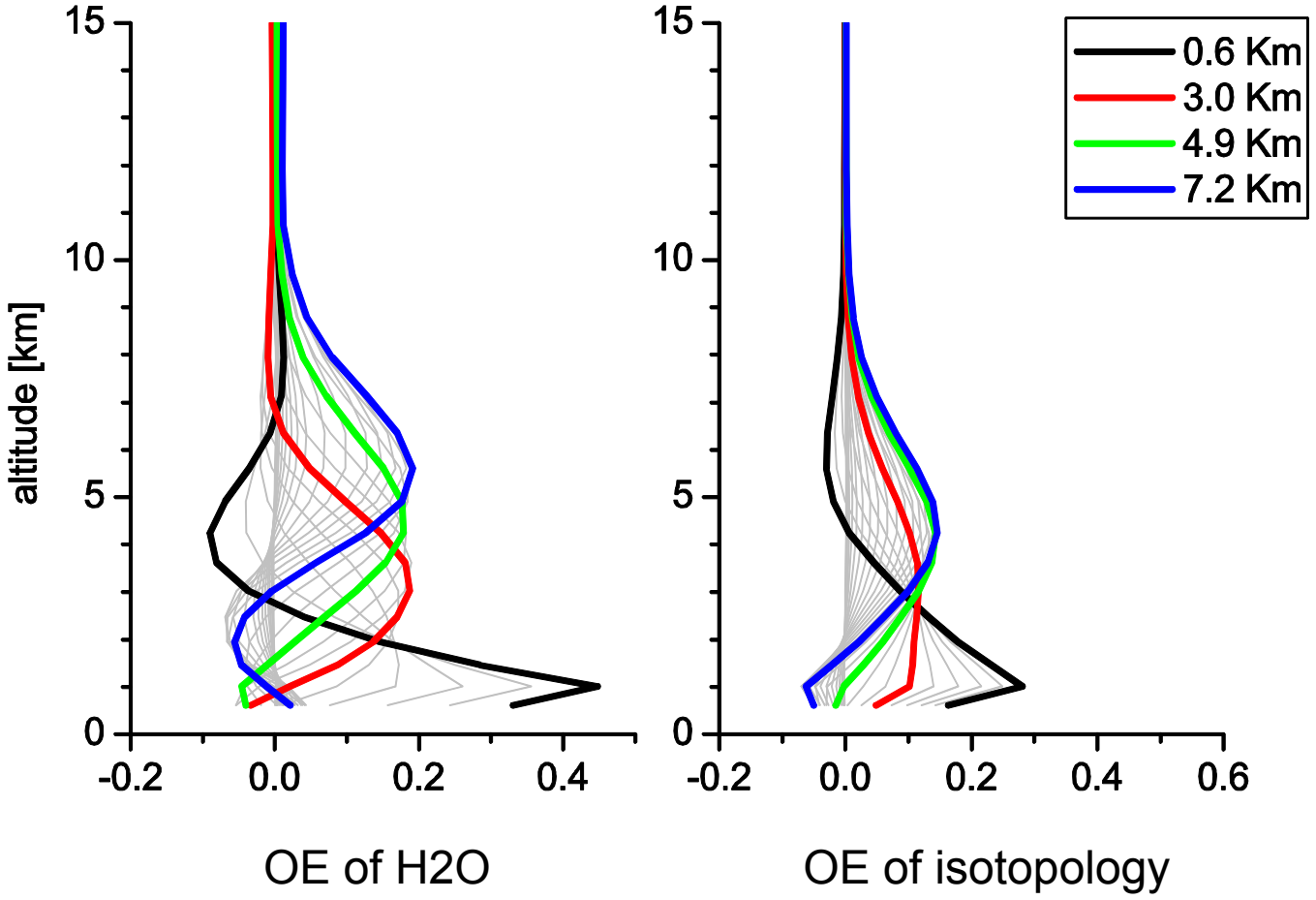
(2)!Optimal estimation of water vapour isotopology state:

-! Quasi no humidity interference to δD, i.e. δD and H2O are independently retrieved

-! Same avks for humidity and δD (DOF:1.7)

APPENDIX: Typical averaging kernels for all ten stations

Eureka, 80.1°N



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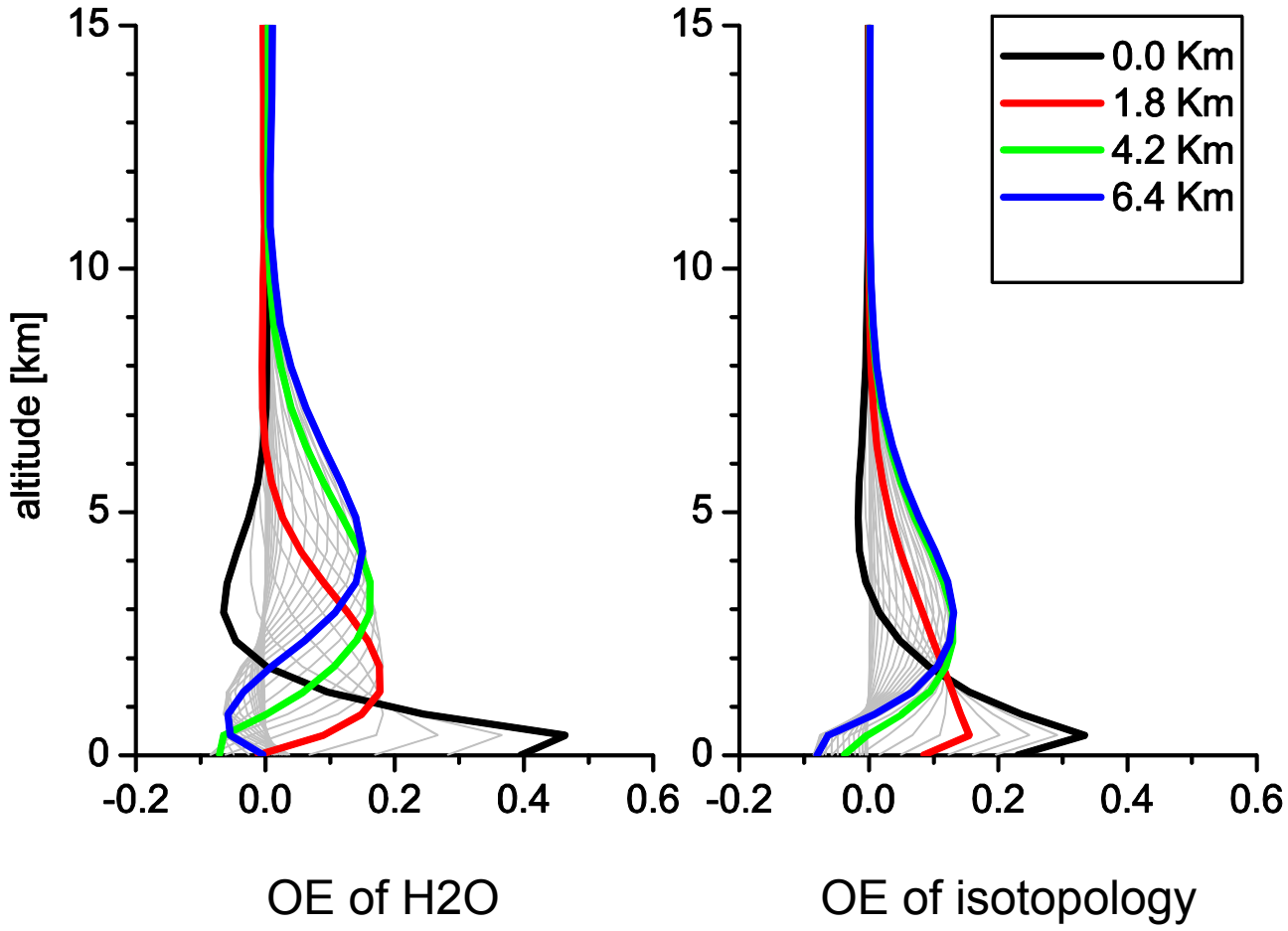
Ny Ålesund, 78.9°N



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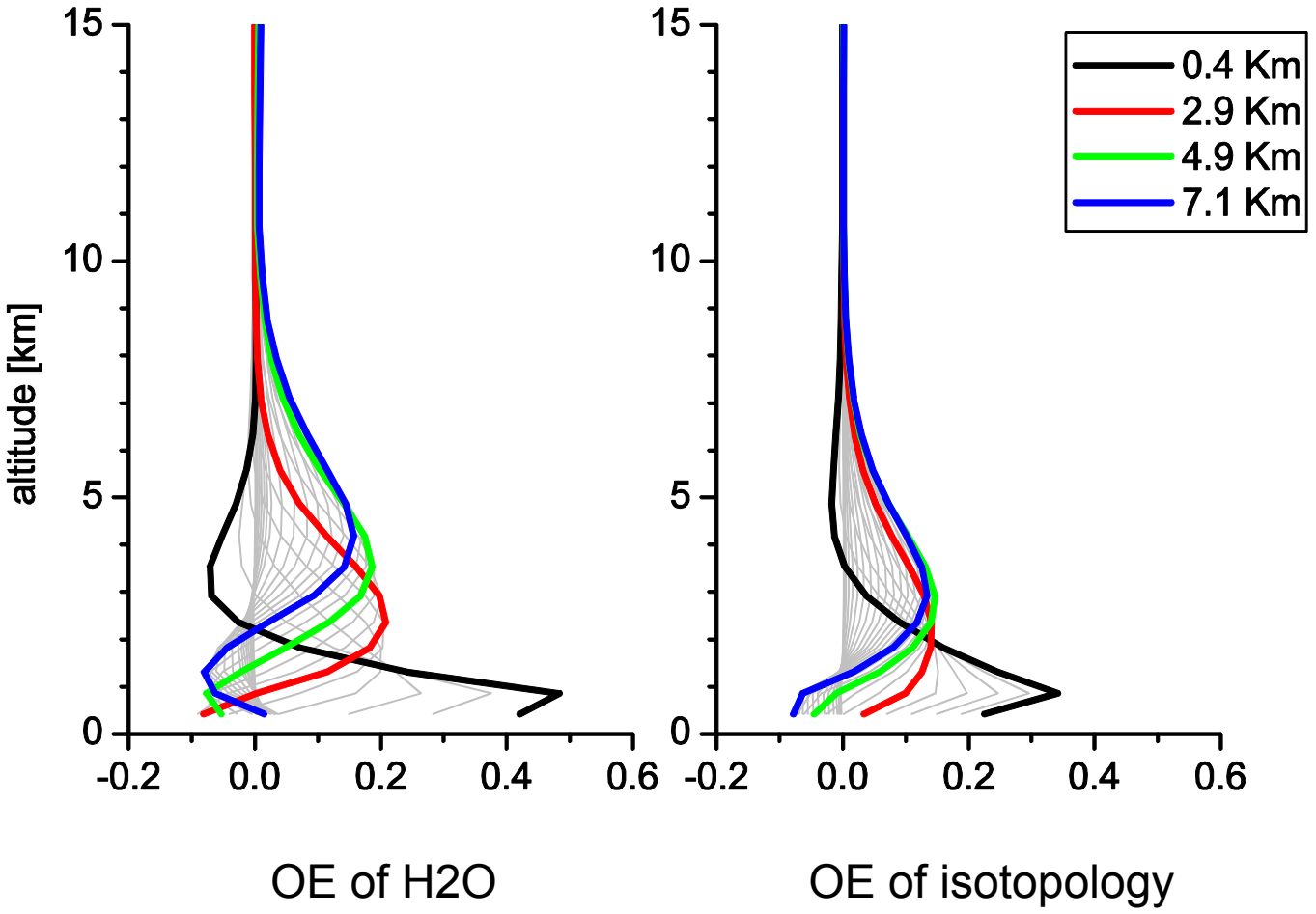
Kiruna, 67.8°N



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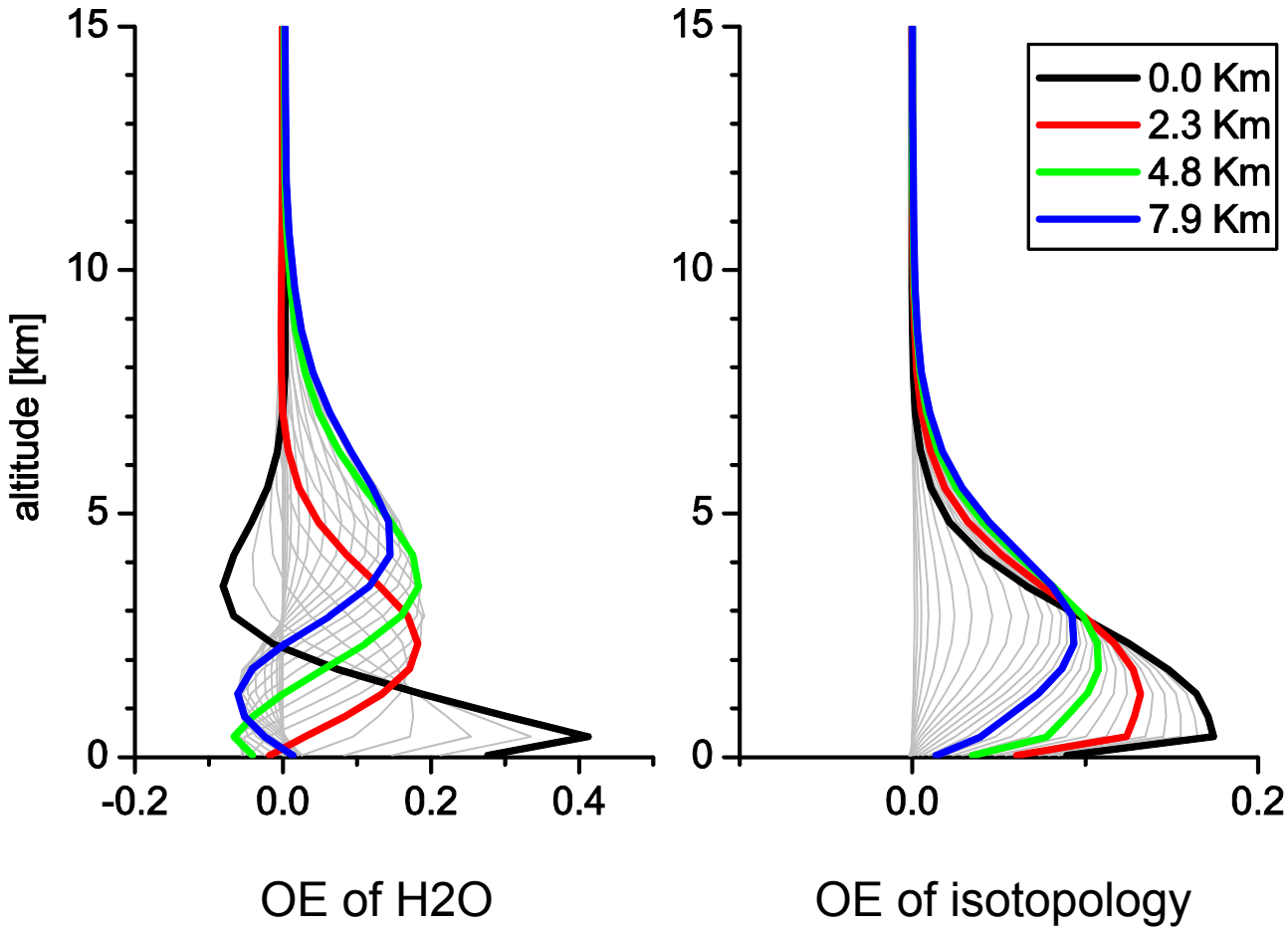
Bremen, 53.1°N



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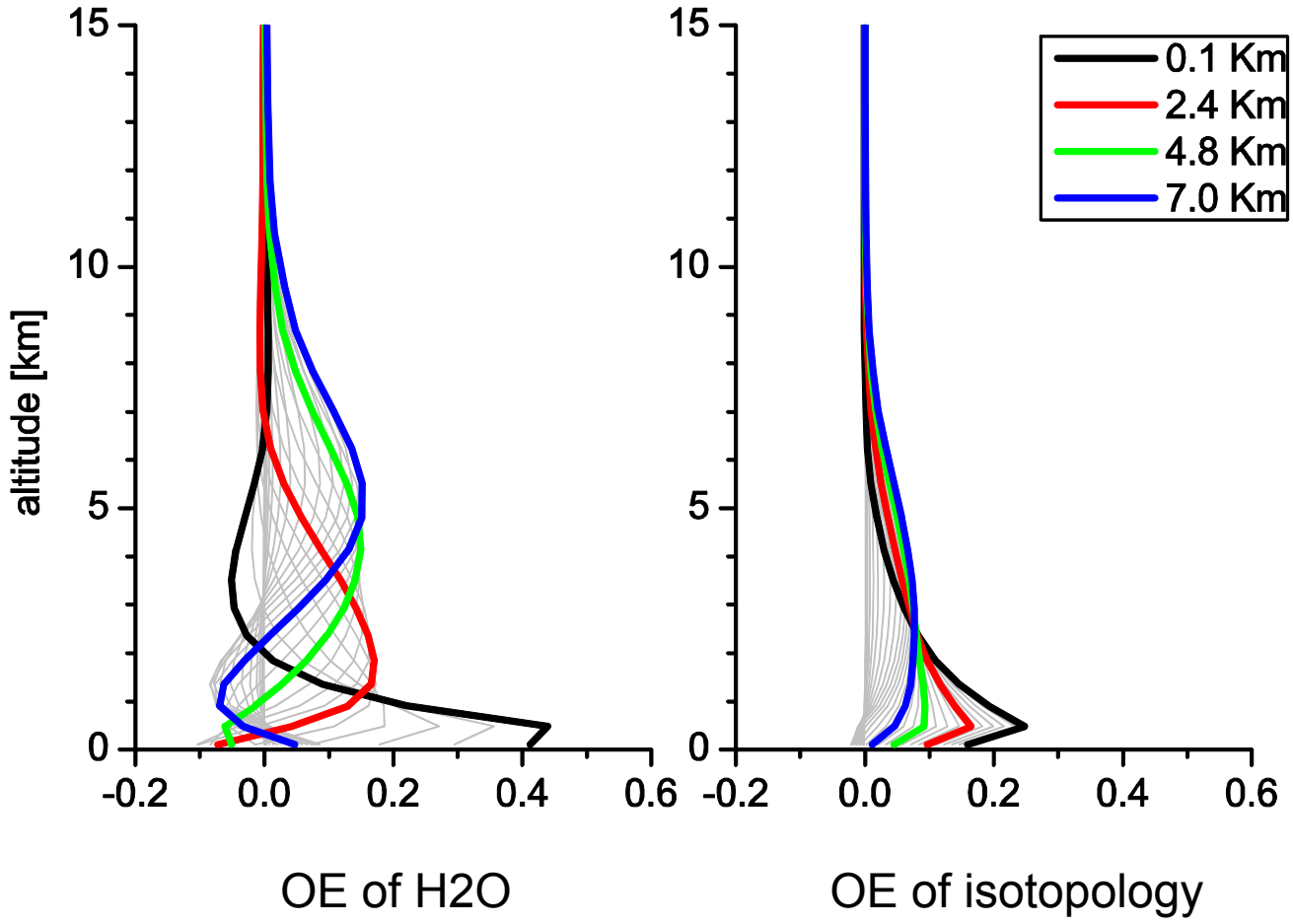
Karlsruhe, 49.1°N



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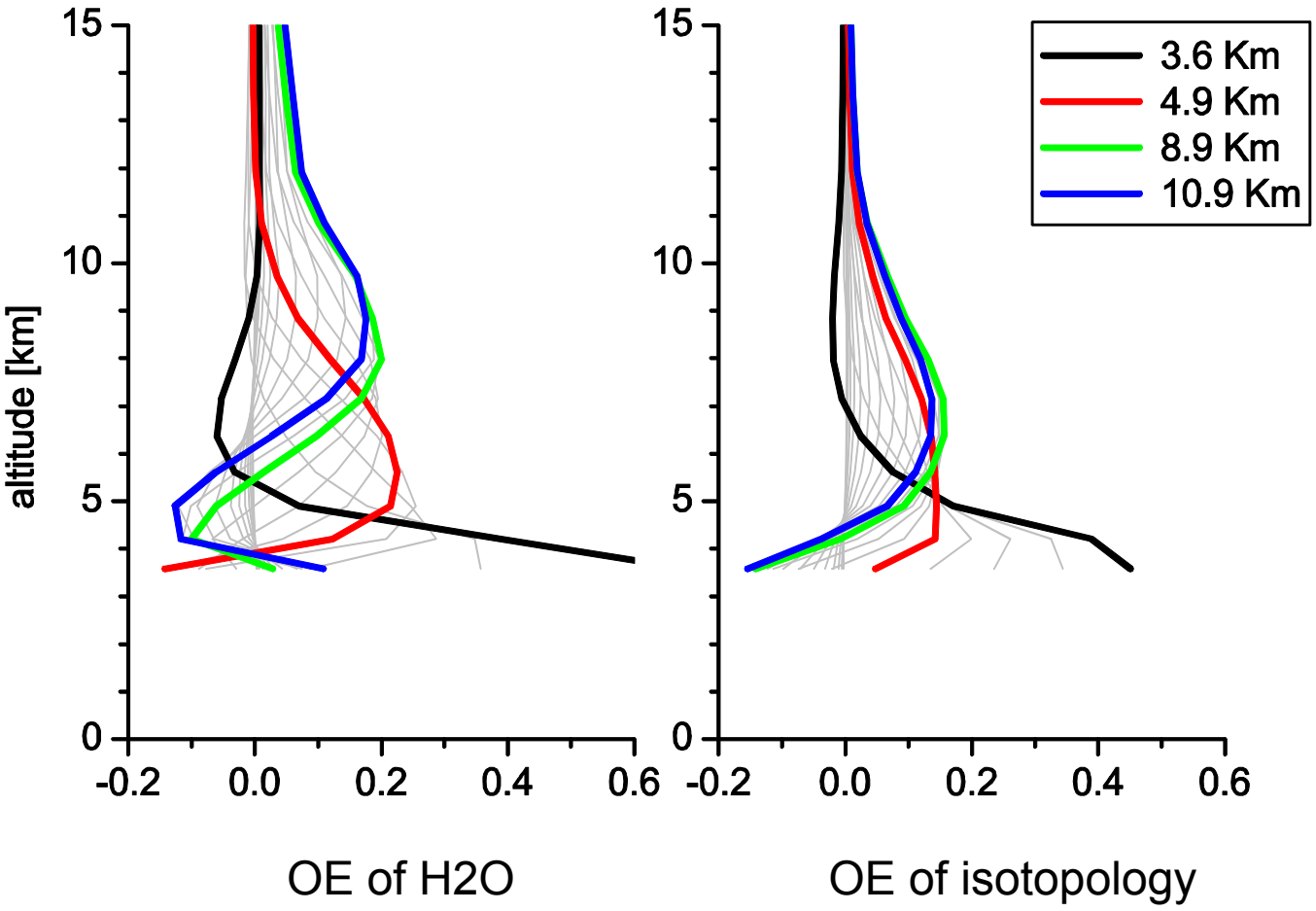
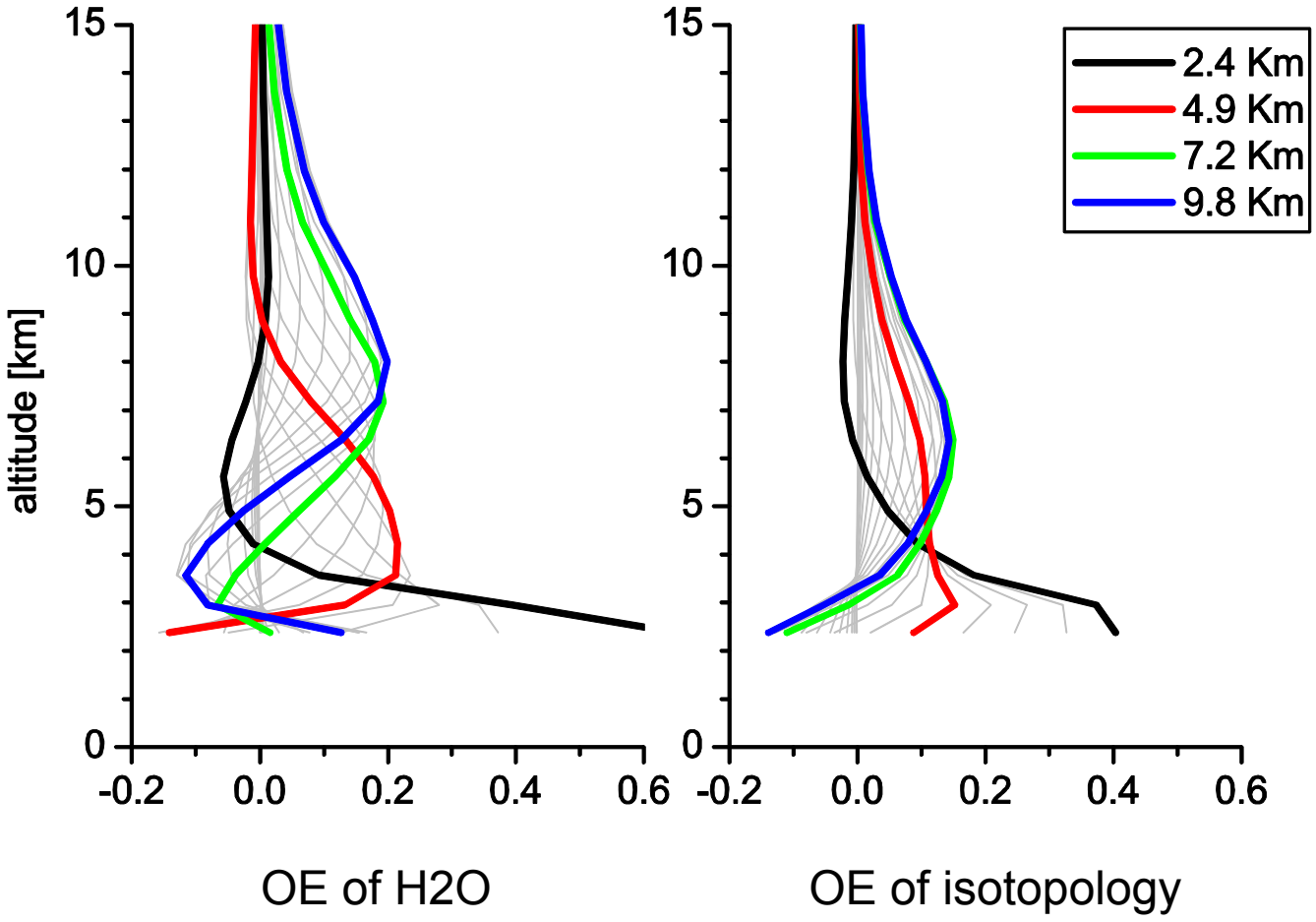
Jungfraujoch, 46.6°N



Izaña, 28.3°N


15
10
5
0
altitude [km]
-0.2
0.0
0.2
0.4
0.6
2.4 Km
4.9 Km
7.2 Km
9.8 Km
OE of H2O
OE of isotopology

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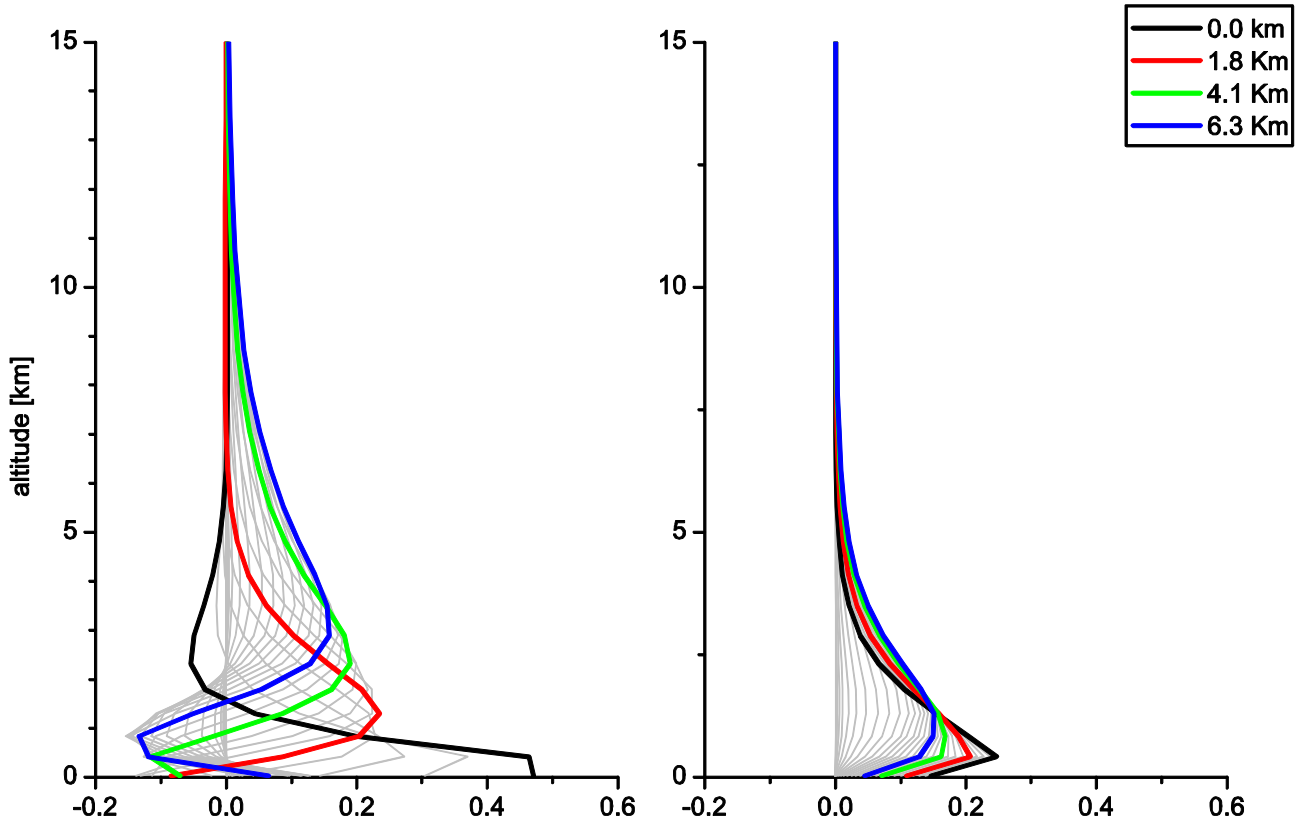
Wollongong, 34.5°S



OE of H2O

OE of isotopology

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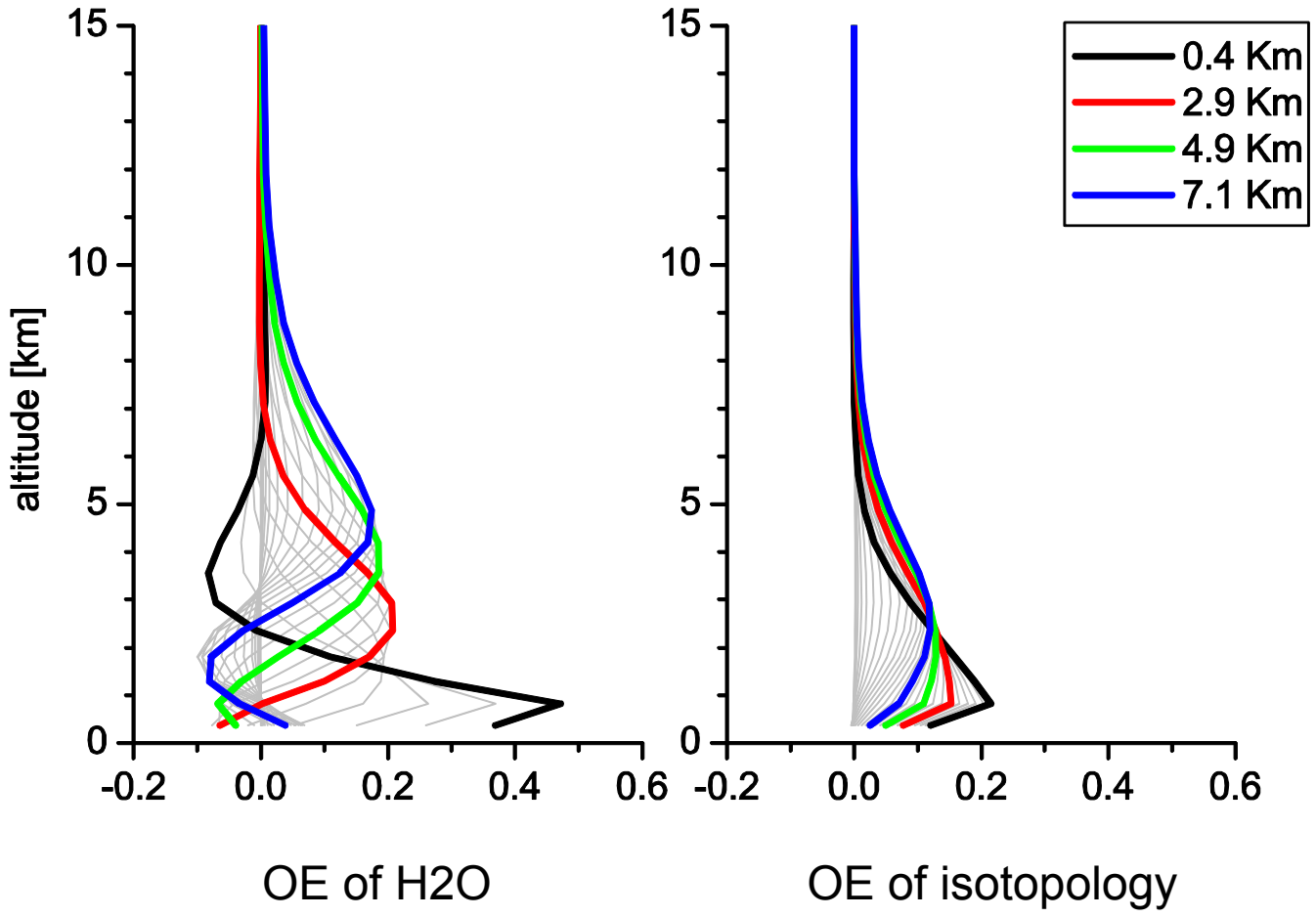
Lauder, 45.1°S



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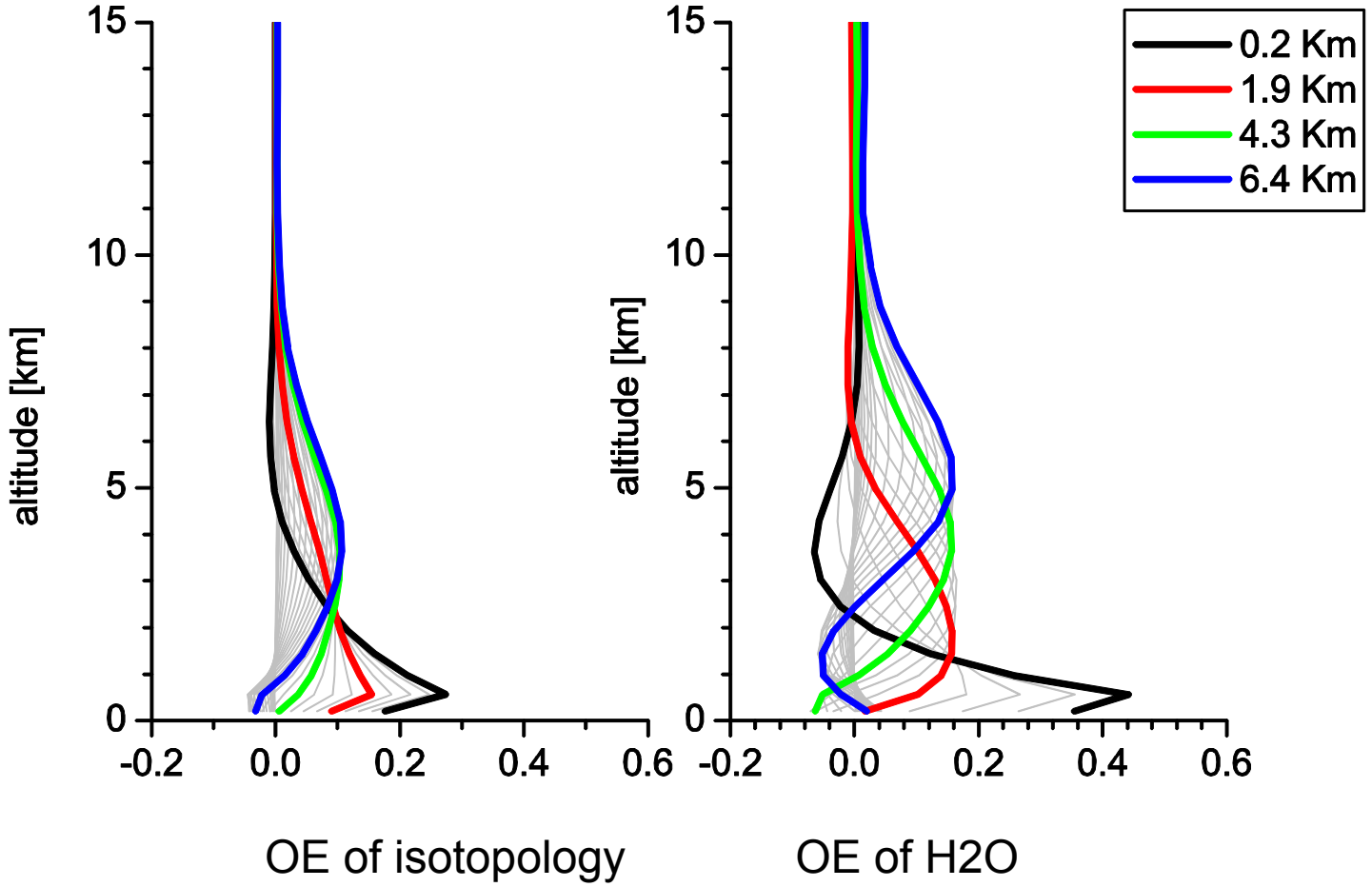
Arrival Heights, 77.8°S



Scientific conclusions + outlook

-! We generated a tropospheric water isotopologue climatology (multi-year mean + multi-year annual cycles) at ten globally distributed sites.

-! We compared the observed climatalogy to a modeled climatology:

(1)!Model is generally too dry in the lower troposphere and too wet in the middle/upper troposphere.

(2)!The isotopologues reveal probable model deficits concerning humidity transport pathways to the high latitudes and the middle/ upper troposphere.

(3)!The isotopologues reveal probable model deficits concerning the annual tropospheric humidity cycle: in the middle troposphere we observe a significant difference between the winter-to-summer and the summer-to-winter transition (similar humidity levels but different isotopic composition), which is not fully captured by the model.

-! Outlook:

(1)!Analyse isotopologue variability wrt backtrajectories, synoptic situations, etc.

(2)!Investigate the observation-model disagreements: compare to different models, compare to different model control runs, etc.