



Materials Science & Technology

Université
de Liège



Achievements in WP5

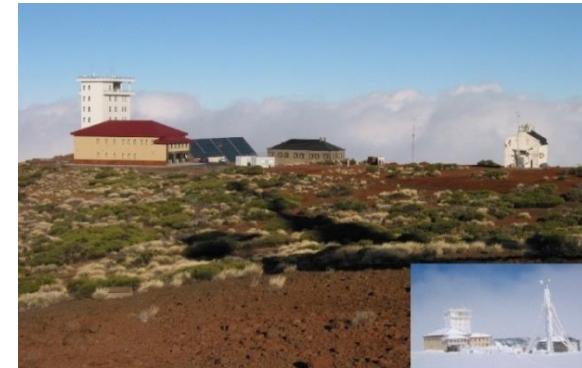
Stephan Henne, Empa

Contributions from BIRA-IASB, INTA, ULg, KIT, AEMET

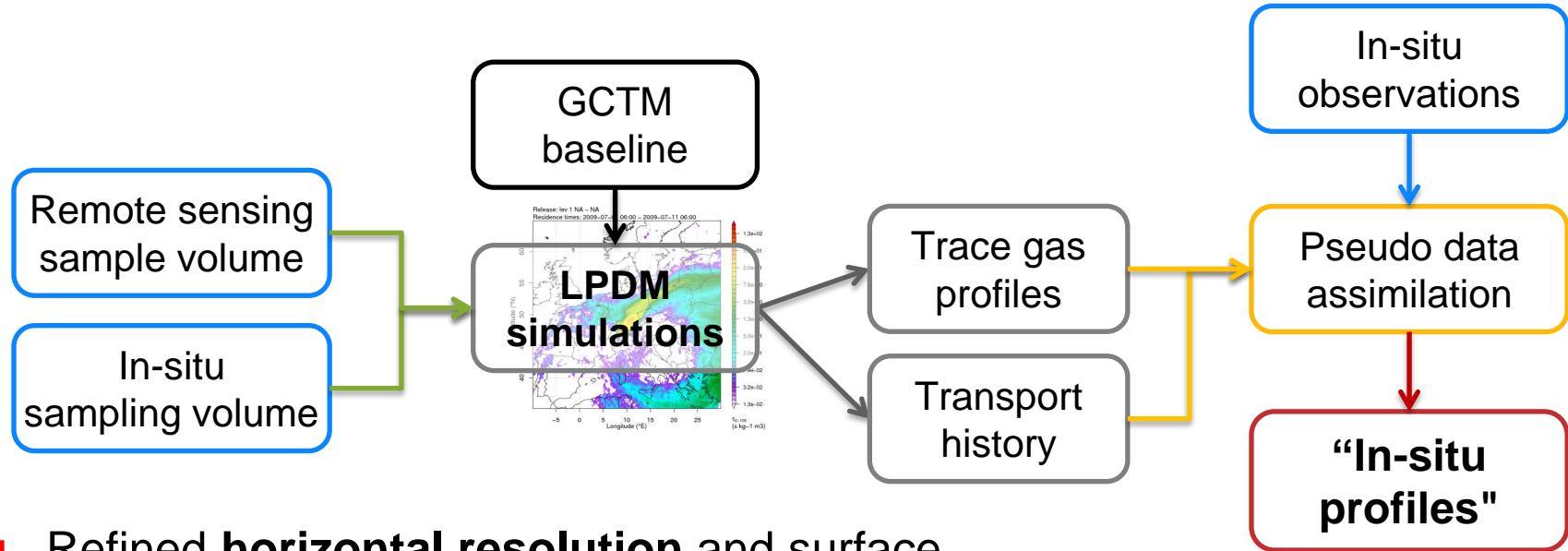
WP5: Validation and integration of tropospheric composition measurements

Main objective

- Further validate NORS products at two demonstration sites (**Jungfraujoch** and **Izaña**) by linking them to **surface in-situ** measurements
- **Surface in-situ**
 - Very good **accuracy, traceability (SI)**
 - **Collocated** with remote sensing sites
 - **Continuous** observations
- **Difficulties of comparison**
 - **Representativeness**
 - **Sensitivity of remote sensing**
 - Individual partial columns not independent
 - Apply **averaging kernel (AVK)**
- **NORS**
 - Characterise **representativeness** of different sampled air masses
 - Construct **calibrated “in-situ profiles”** by blending surface observations with model profiles



In-situ Profile vs. Direct Model Comparison



- Refined **horizontal resolution** and surface representation
- Refined transport to specific sampling volume: reducing the **representativeness error** that arises in grid box models
- **Transport history** accessible for each sub-column
- Separation into background and pollution contribution
- Direct relaxation towards surface data only for sub-columns with similar air mass history

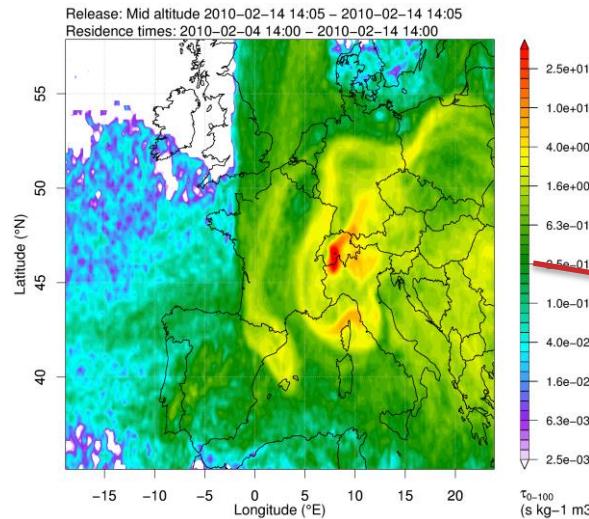
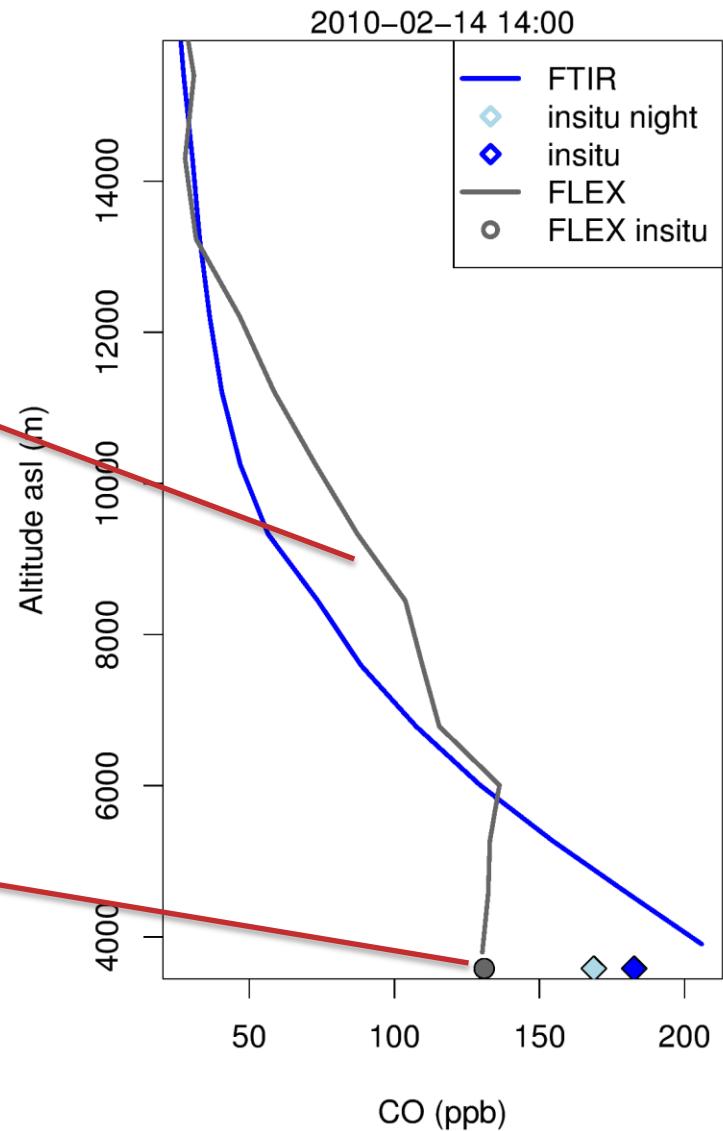
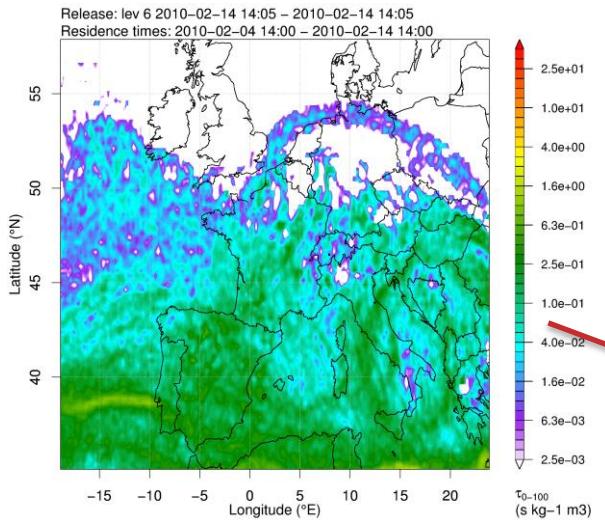
D5.1

Limitations

- Method not based on a rigorous mathematical framework
- Currently, method does not include uncertainty propagation from surface in-situ to reference profile
- Method requires a model simulation that is locally not too biased
 - Model validation by independent observations required (surface + profile)
 - Model validation + surface correction vs. data assimilation
- Method best for passive tracers (as treated in the LPDM); for reactive species additional tuning may be required
- Validity of profile adjustment not validated

Example Profile: Jungfraujoch, CO

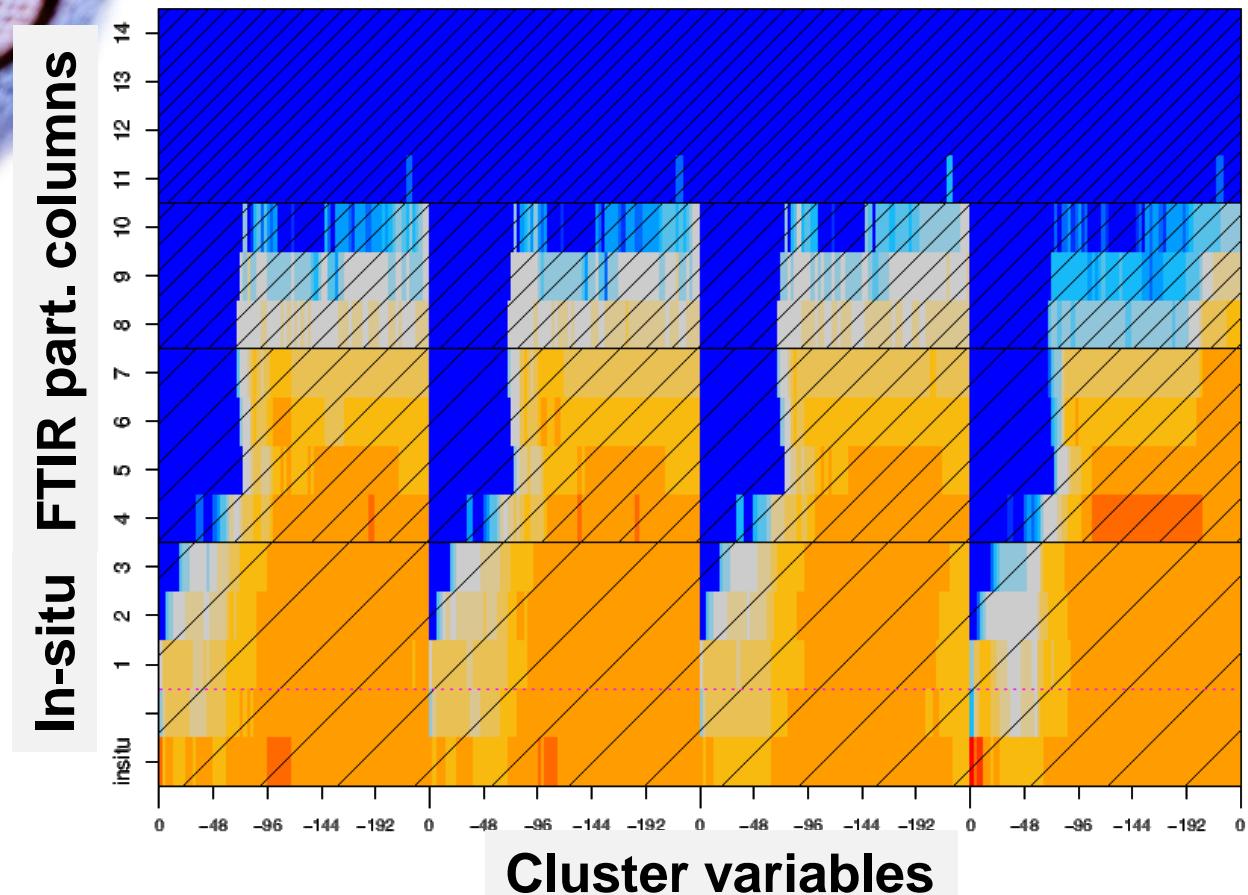
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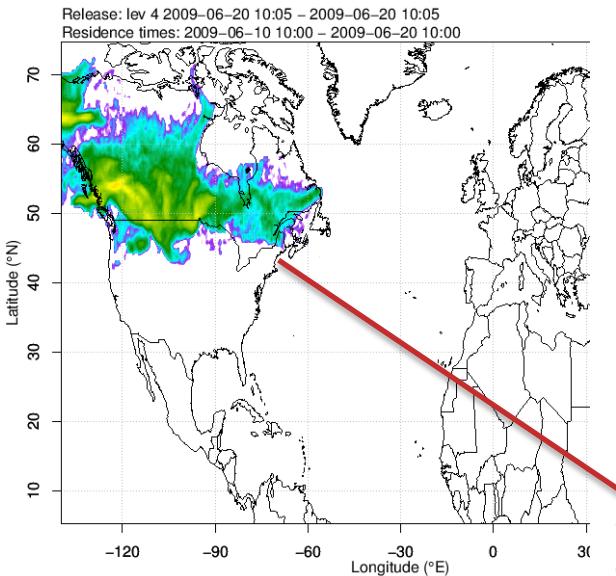
How to Distinguish Atmospheric Layers



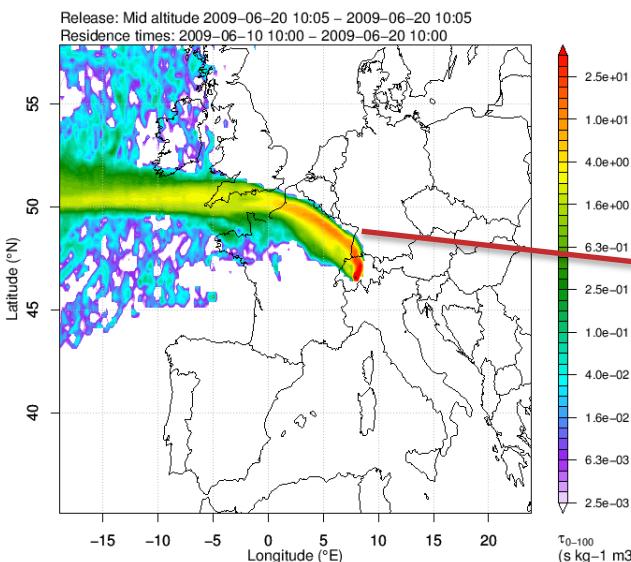
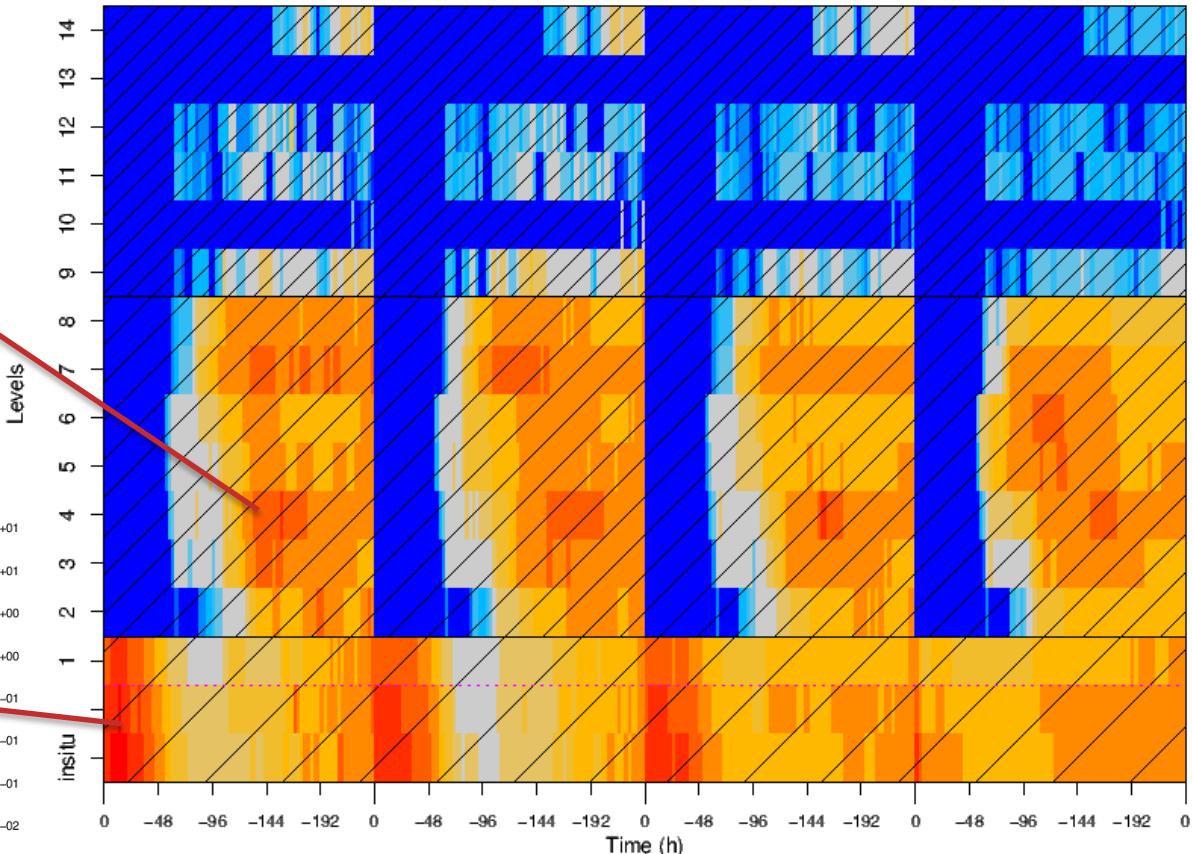
- ## Clustering of FLEXPART footprints
- Surface residence time and emission uptake vs. time
 - Ward Clustering
 - Number of clusters obtained from inter-cluster variance



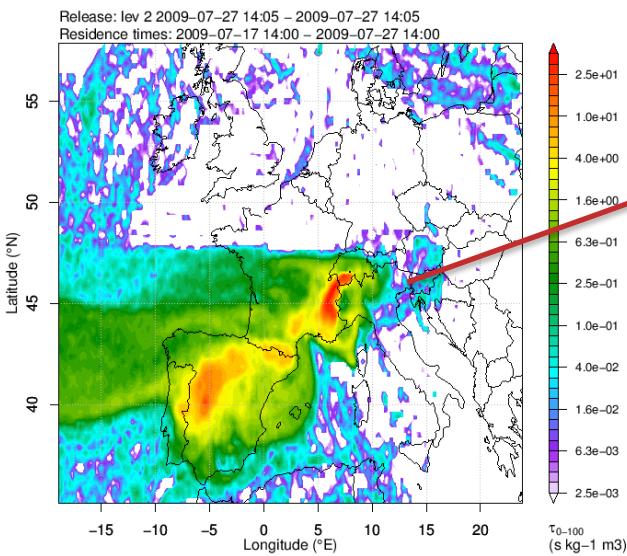
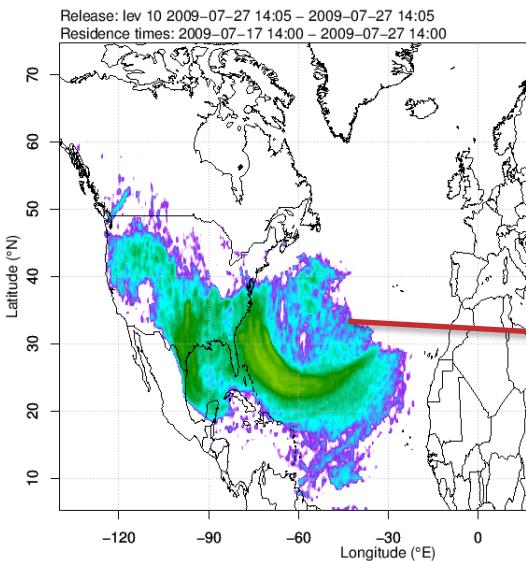
Footprint Clustering: Shallow in-situ Layer



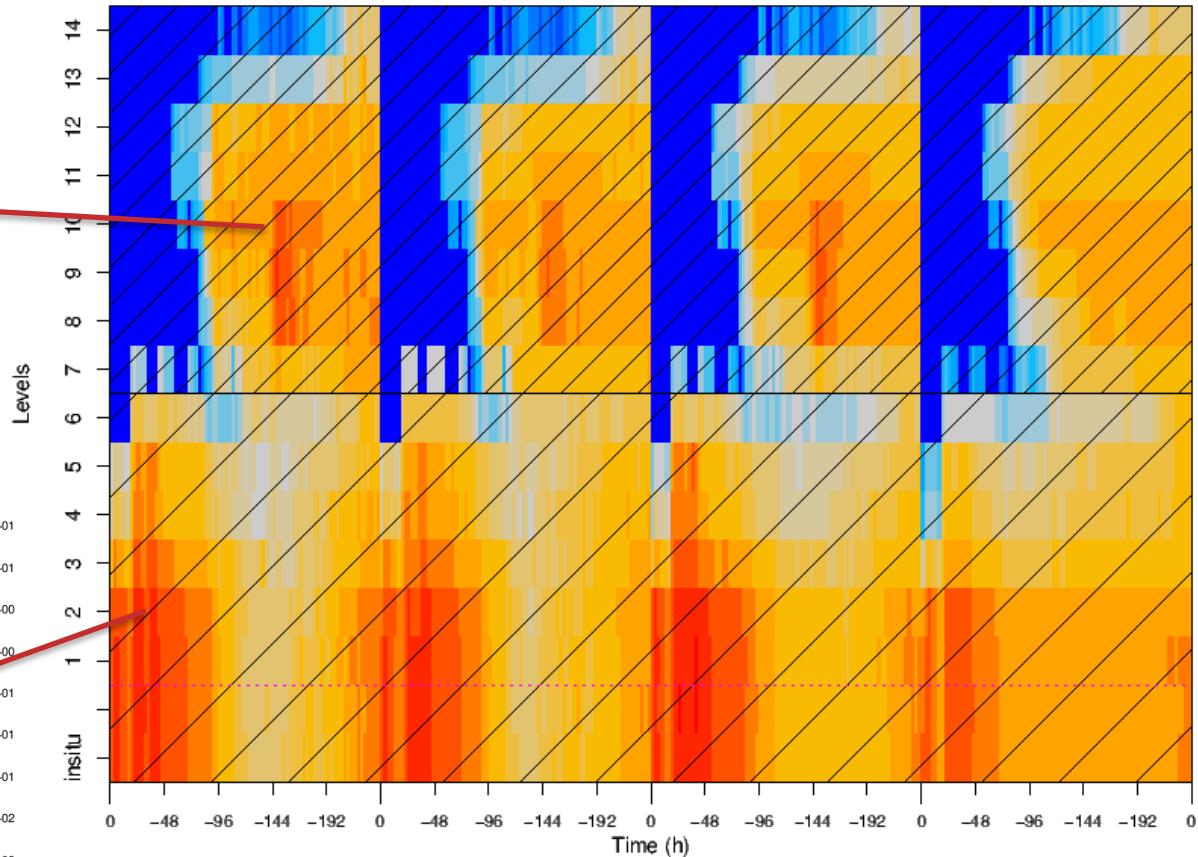
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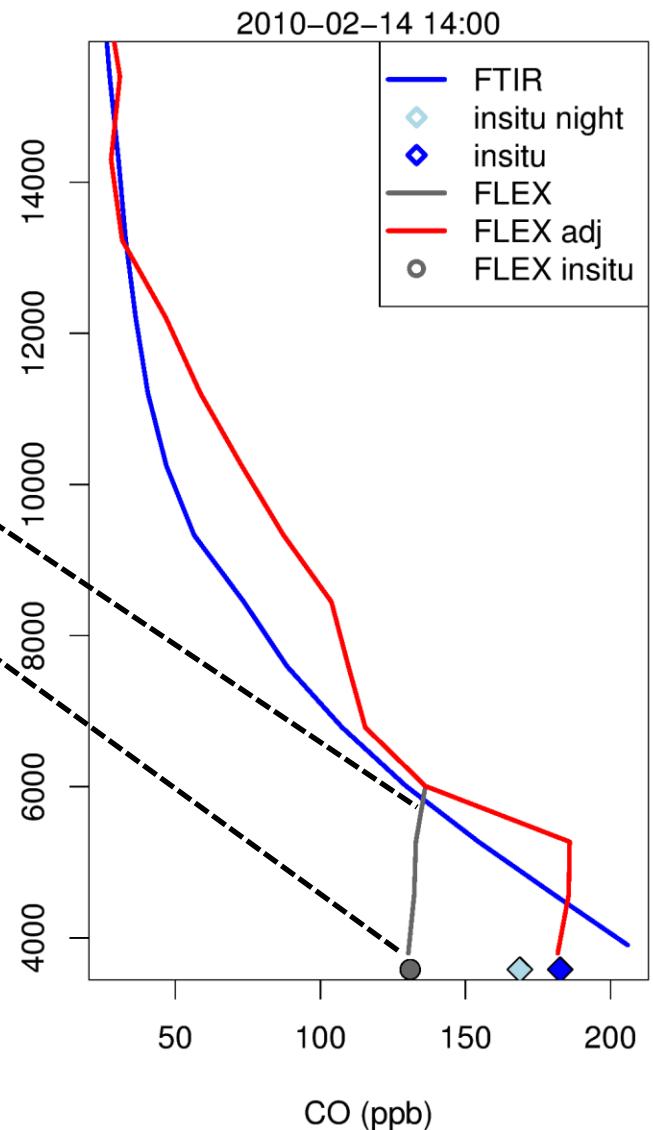
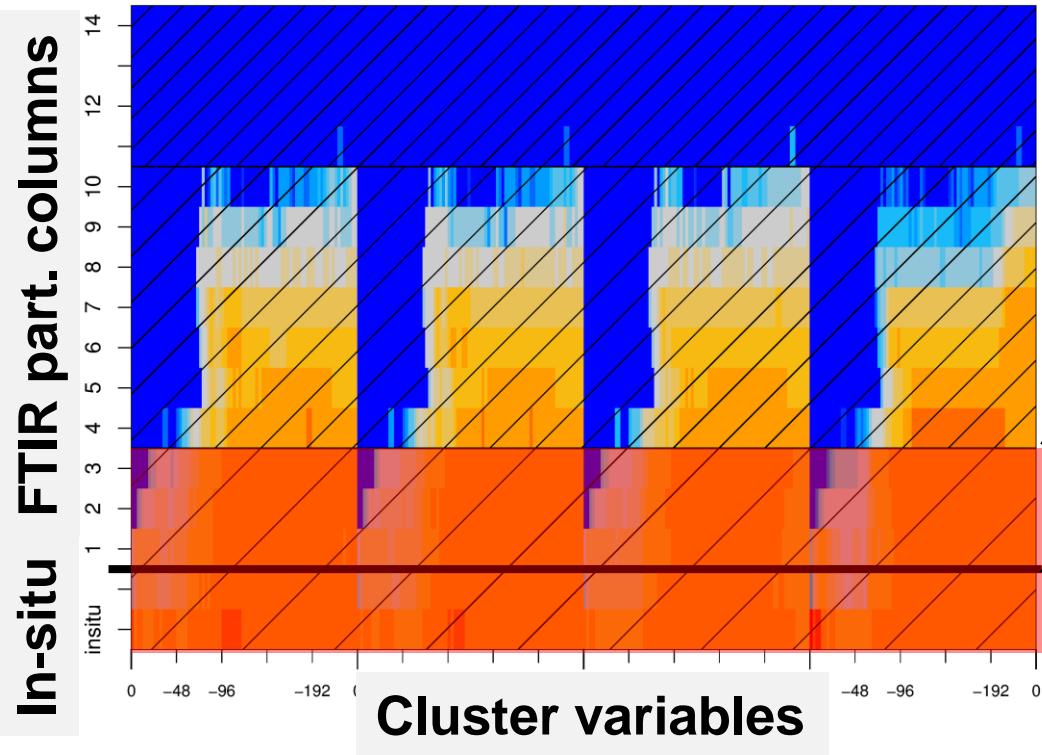
Footprint Clustering: Deep in-situ Layer



2009-07-27 14:00



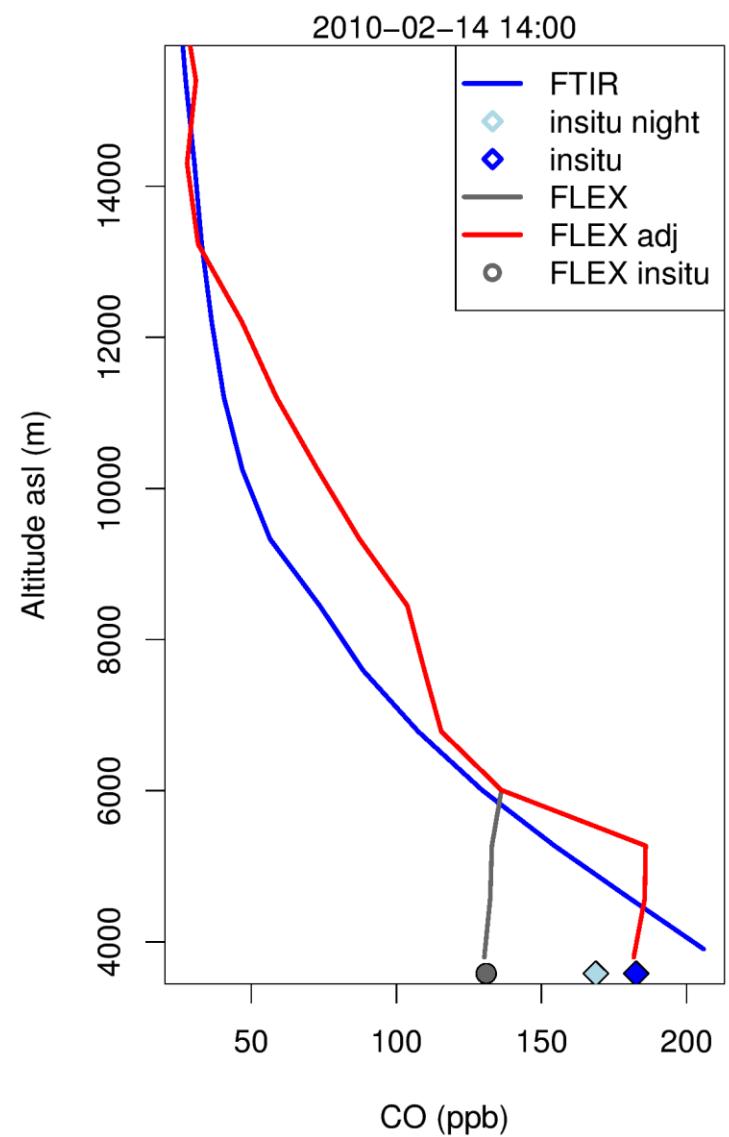
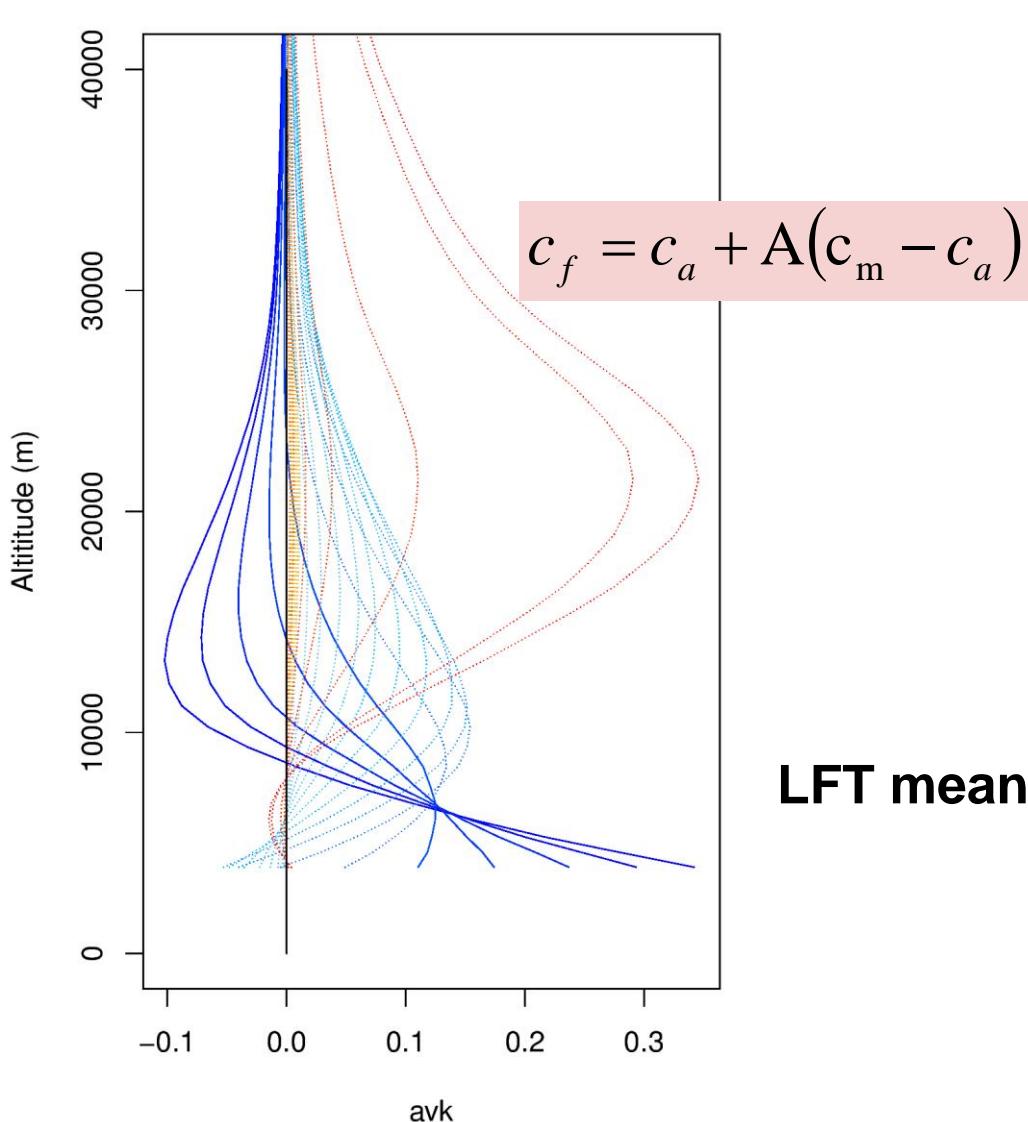
Adjustment of Model Profile



Adjustment

- Separating background and pollution
- Bias correction for background
- Factorial correction for pollution

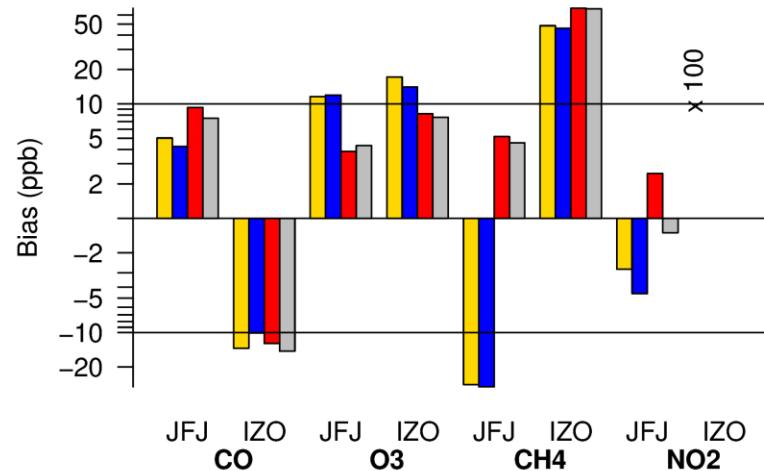
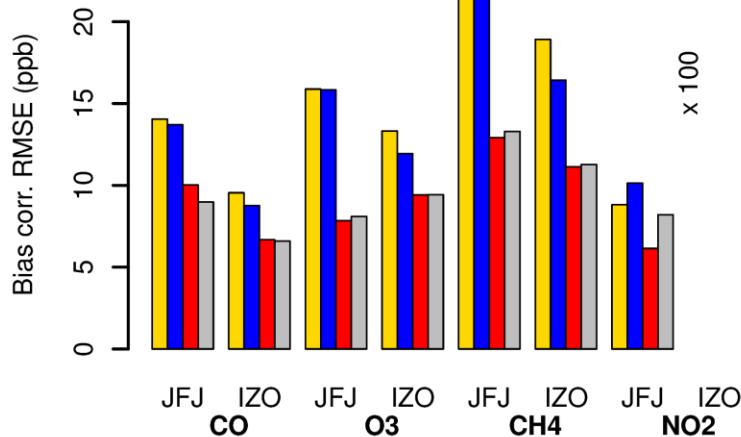
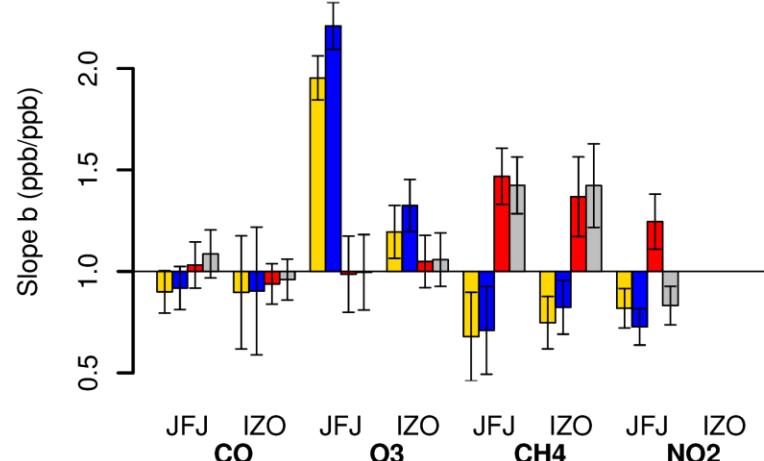
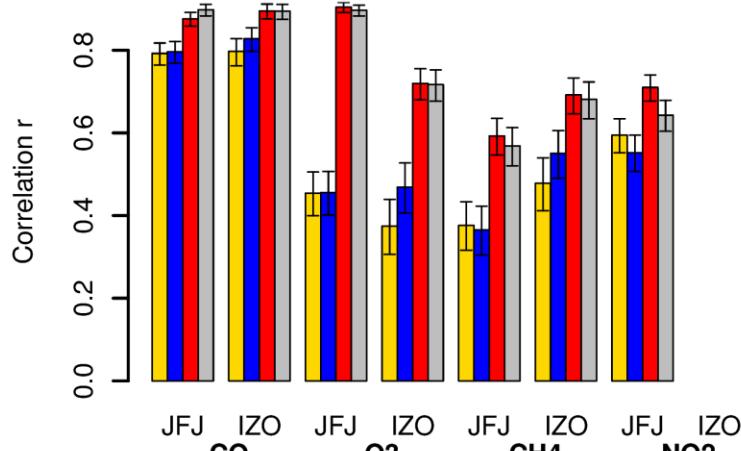
Folding with Averaging Kernel and LFT Mean



Comparison Datasets

Site	Parameter	Instrument	Retrival	Period	GCTMs
JFJ	CO	FTIR	Profile	2009-2011	FLEXCTM, MACC
JFJ	O ₃	FTIR	Profile	2009-2011	MACC
JFJ	CH ₄	FTIR	Profile	2009-2011	FLEXCTM, TM5, MACC
JFJ	NO ₂	MAXDOAS	Profile	2011-2012	MACC
IZO	CO	FTIR	Profile	2009-2011	MACC, FLEXCTM
IZO	O ₃	FTIR	Profile	2009-2011	MACC
IZO	CH ₄	FTIR	Profile	2009-2011	FLEXCTM, TM5, MACC
IZO	O ₃	MAXDOAS	MGA	2011-2012	MACC
IZO	NO ₂	MAXDOAS	MGA	2011-2012	MACC

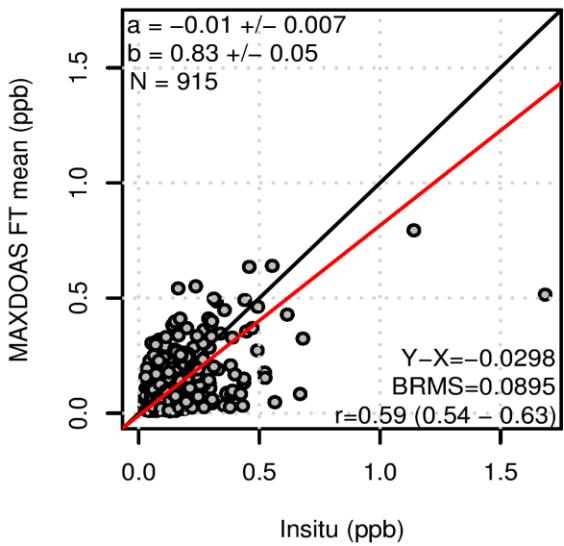
Comparison Statistics: Tropospheric Column (DOF=1)



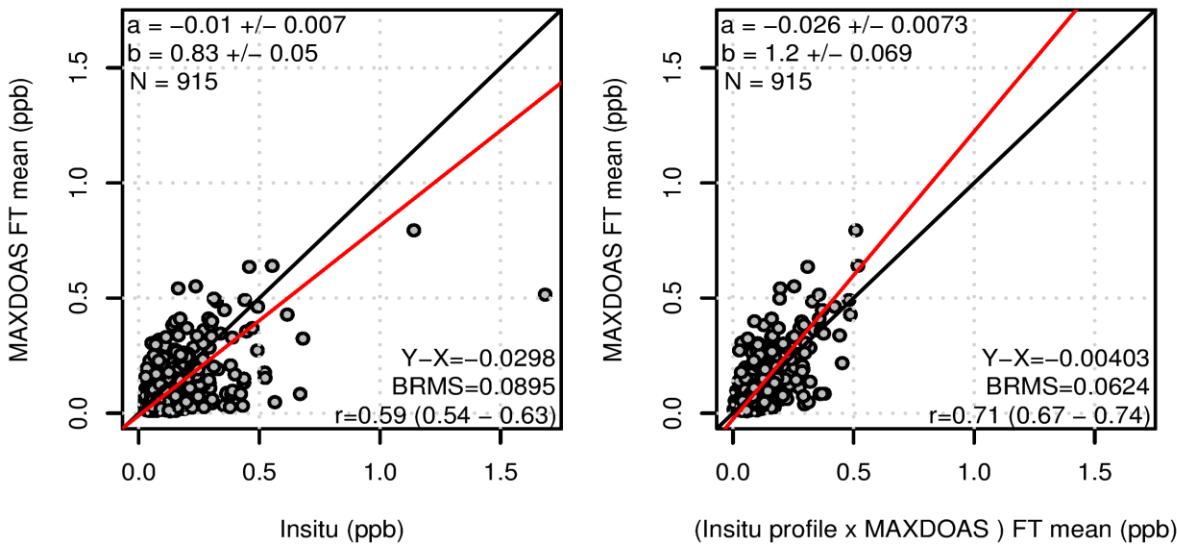
D5.3

NO_2 MAXDOAS Jungfraujoch

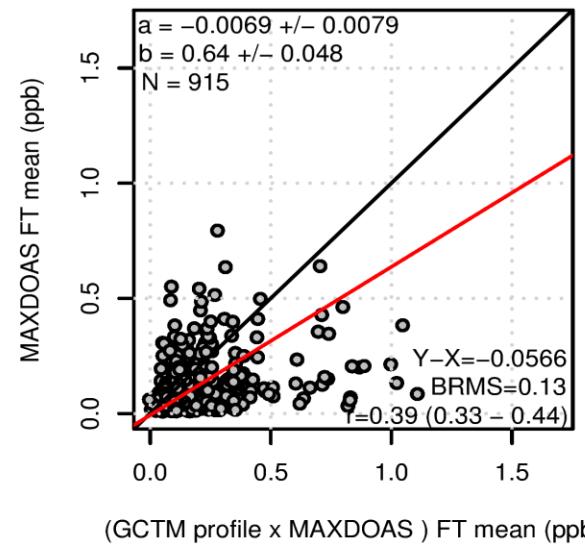
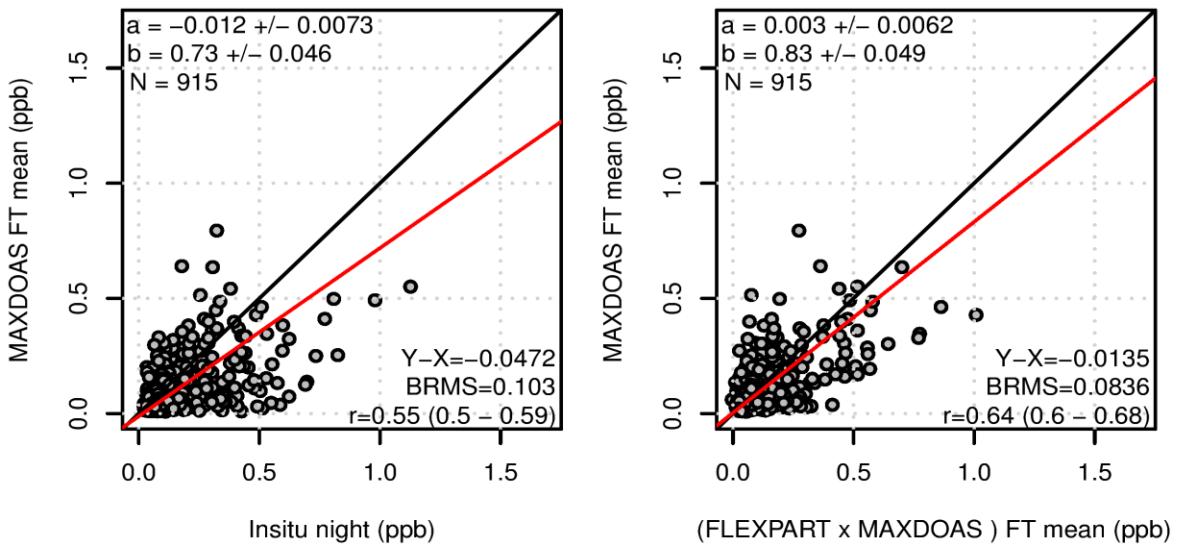
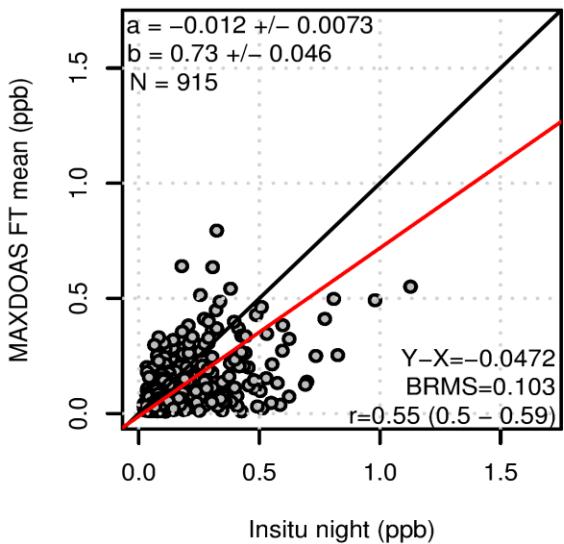
in-situ comparisons

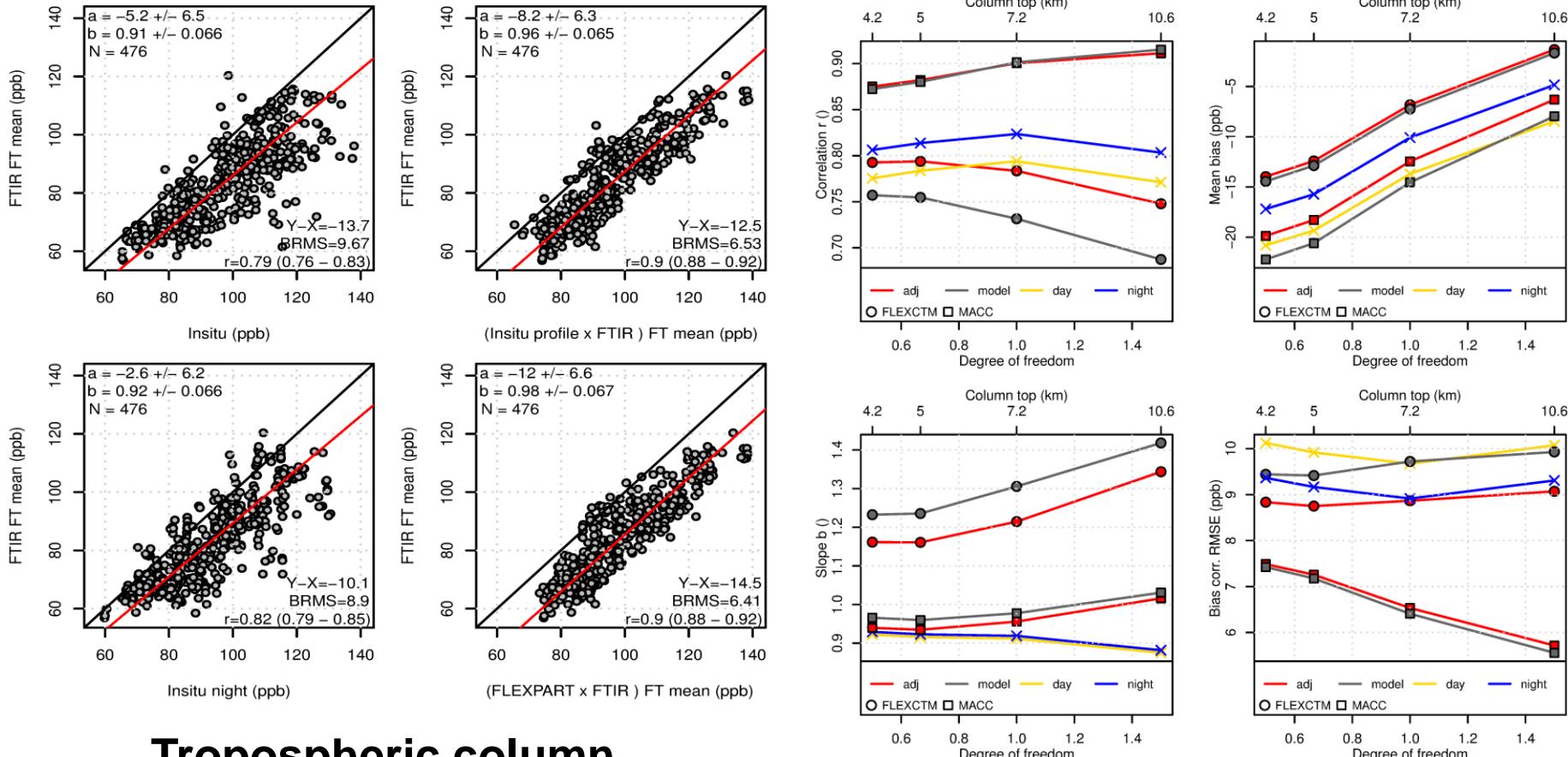


column comparisons



MAXDOAS column up to 4.06 km asl

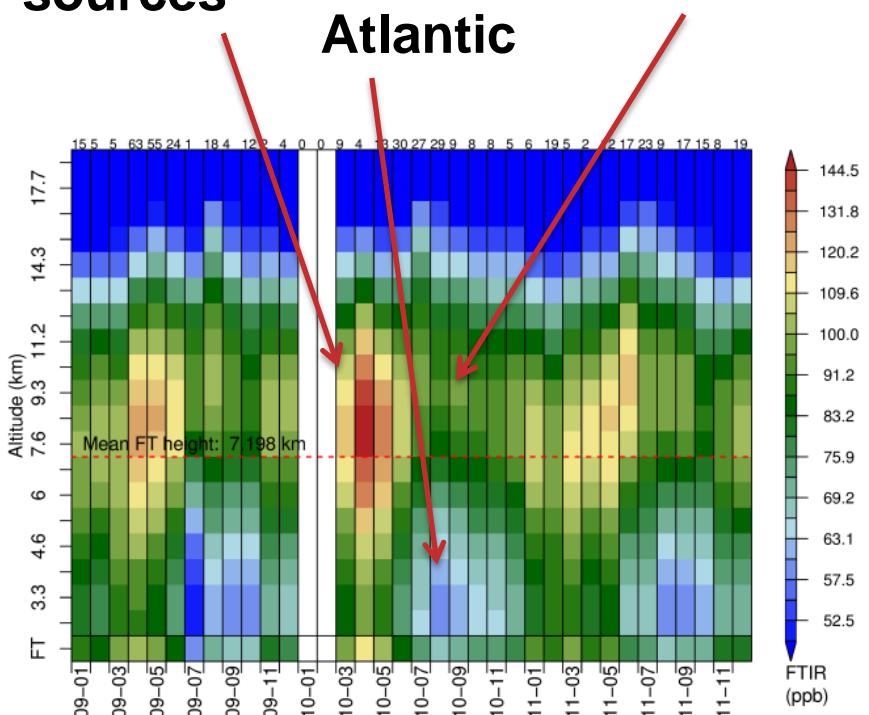




**Tropospheric column
up to 7.2 km asl**

Dependence on column height

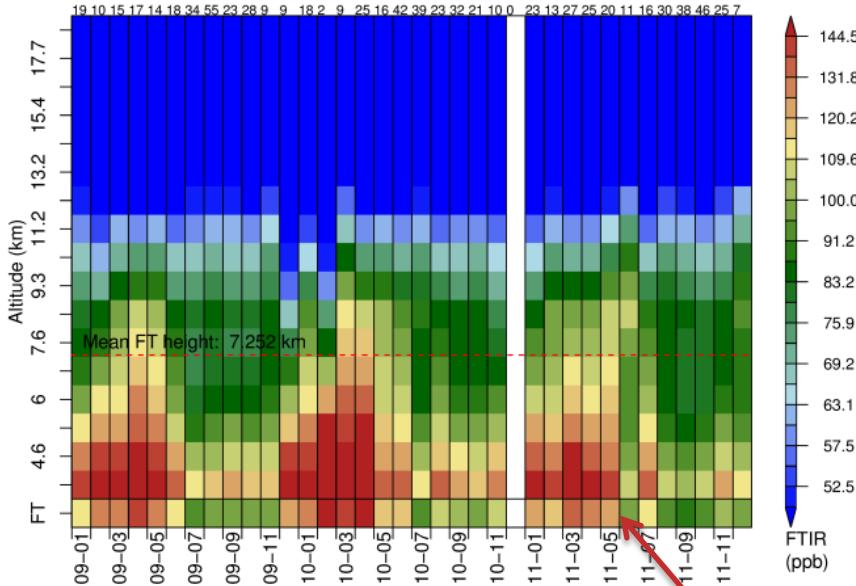
North American sources



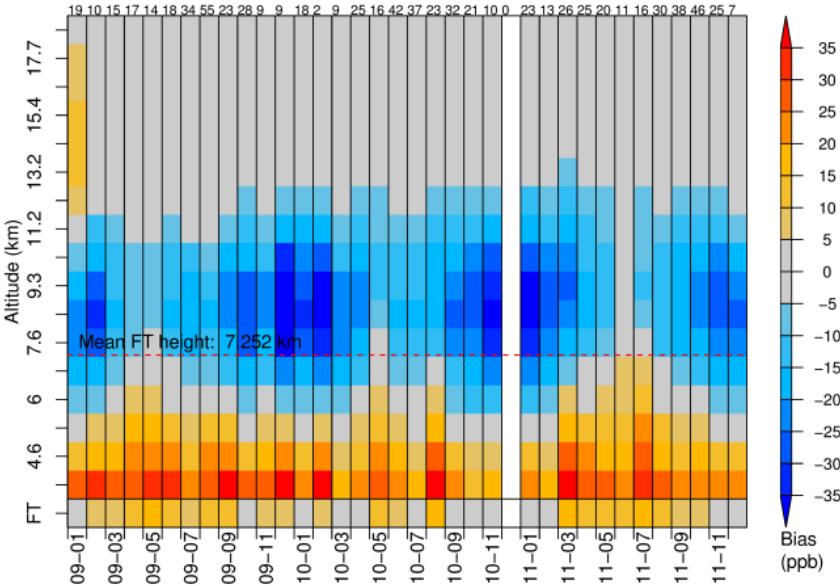
FTIR monthly mean concentrations

http://lagrange.empa.ch/NORS_browser

CO FTIR Jungfraujoch



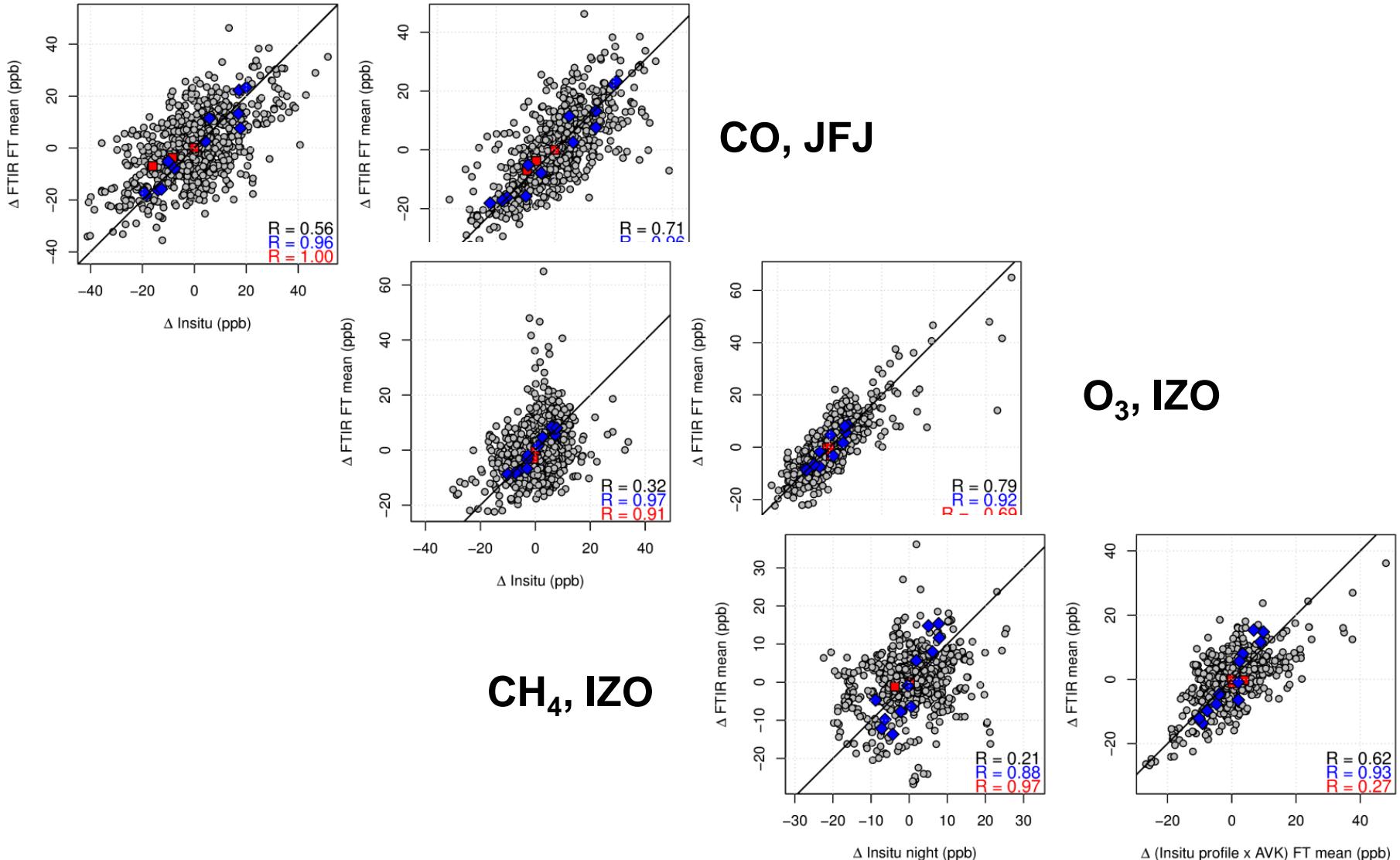
FTIR monthly mean concentrations



FTIR monthly mean bias

European PBL

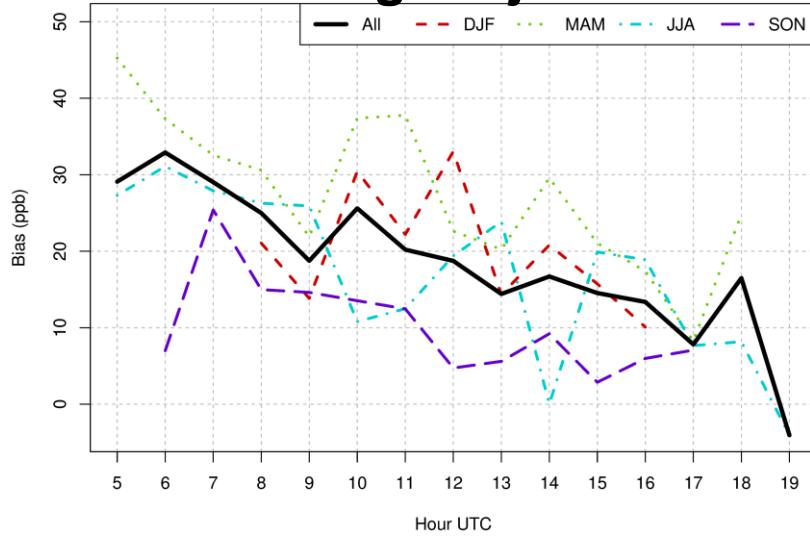
Temporal Variability



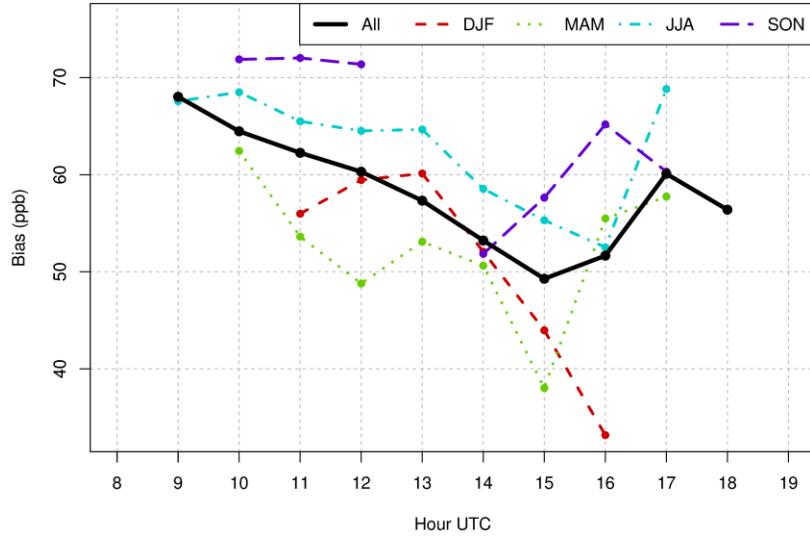
Diurnal Cycle of CH₄ Bias

In-situ

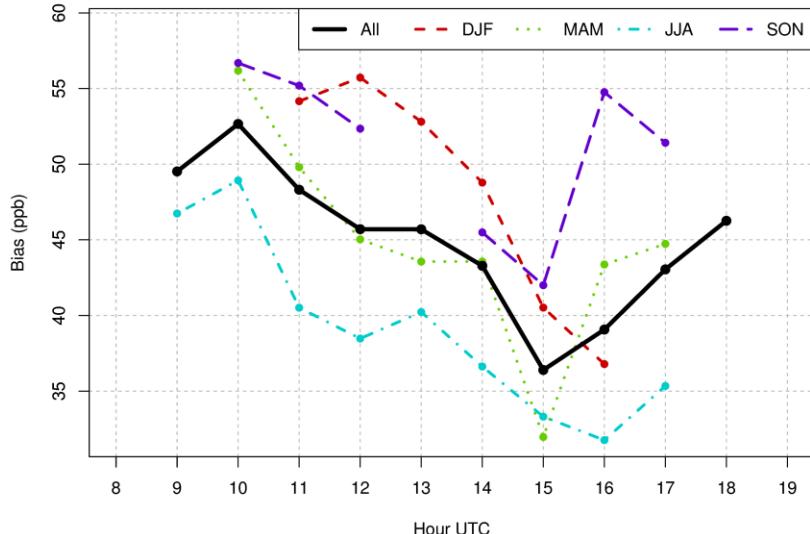
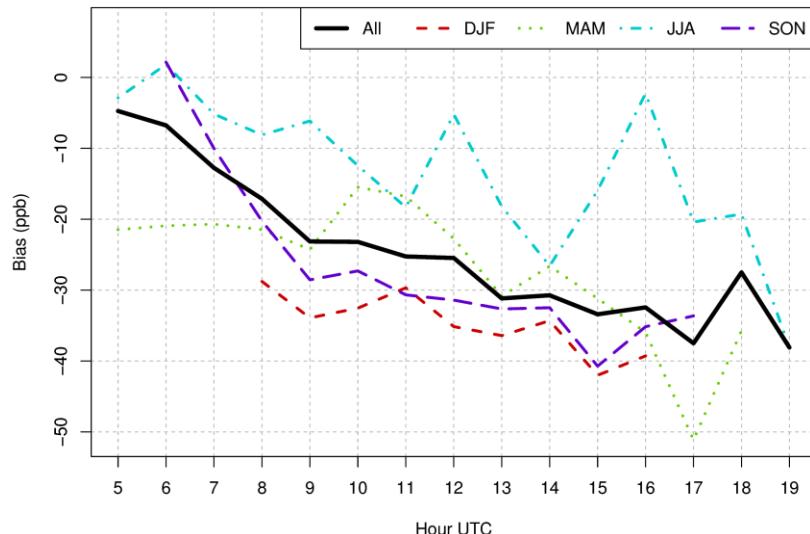
Jungfraujoch



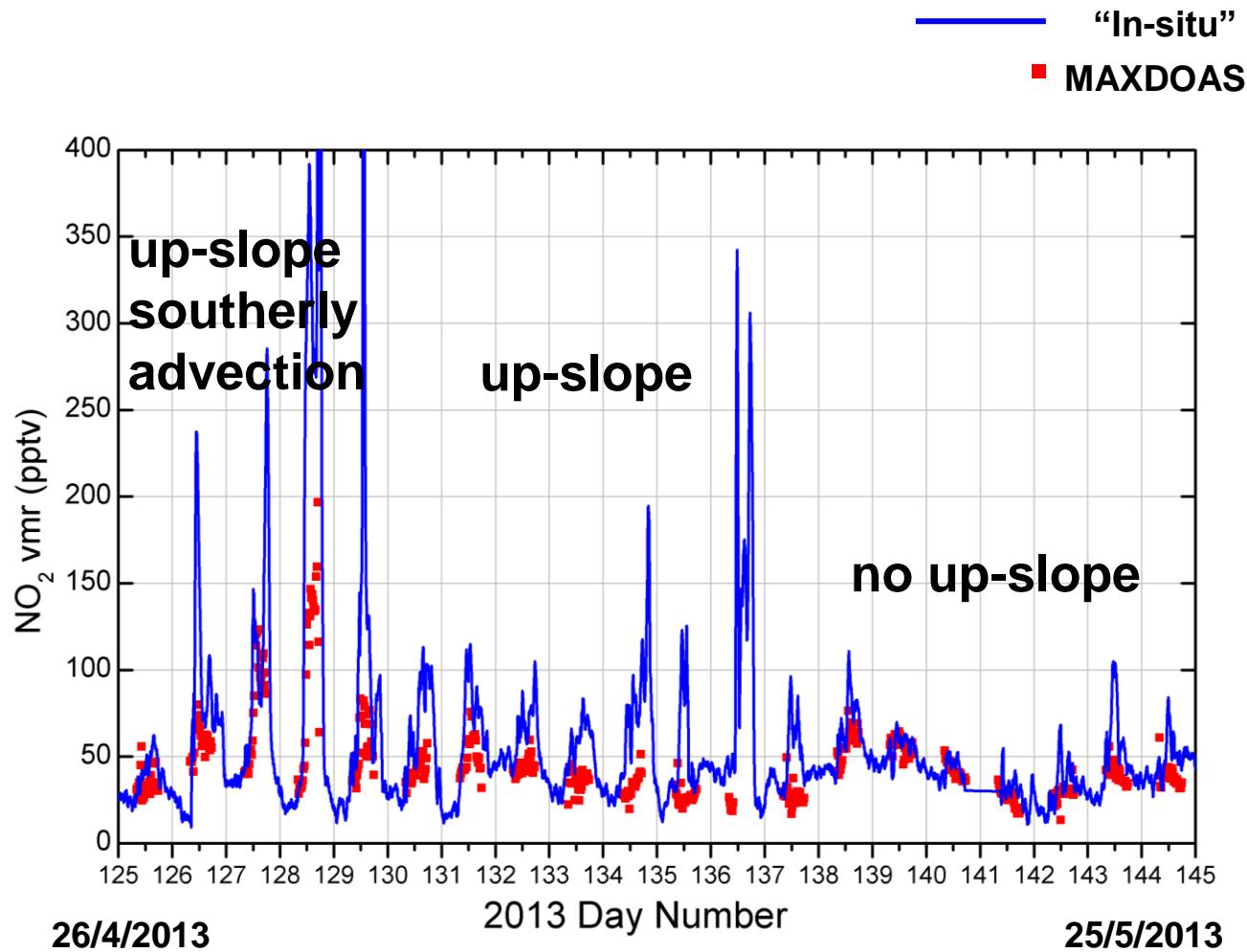
Izaña



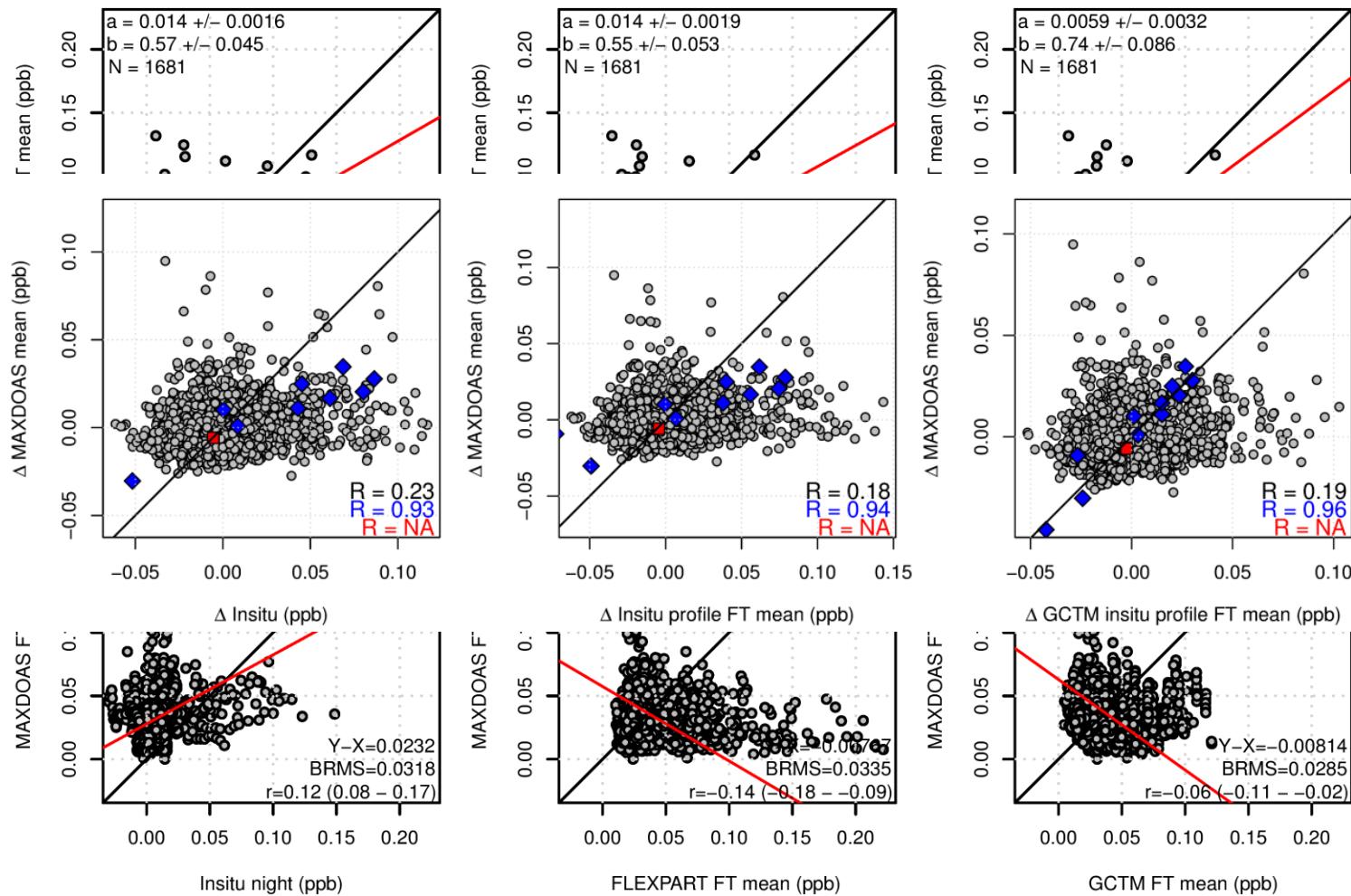
In-situ column



NO_2 MAXDOAS MGA Izaña

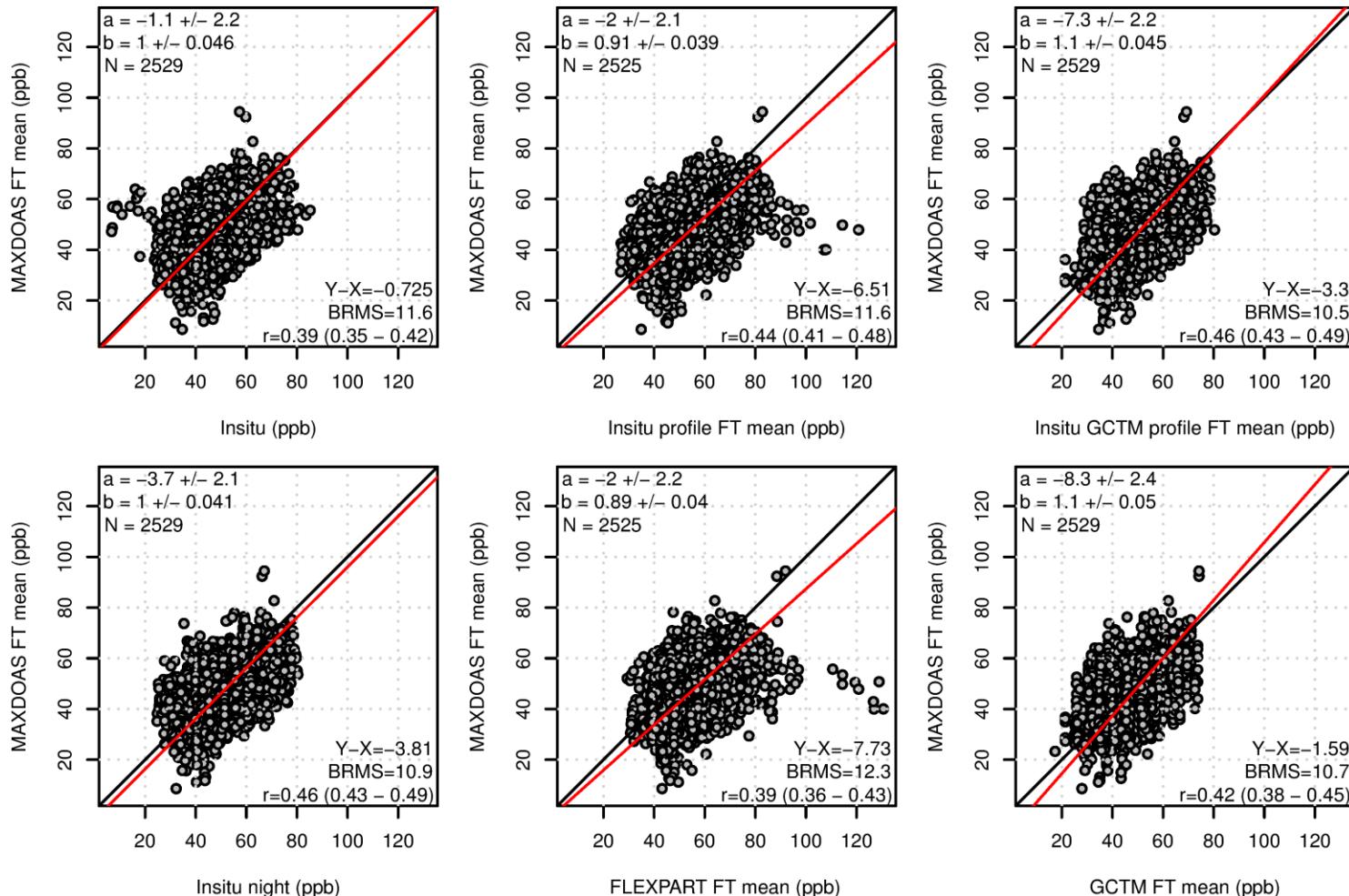


NO_2 MAXDOAS MGA Izaña



In-situ not suited for validation: local influence, detection limit

O₃ MAXDOAS MGA Izaña



**In-situ columns do not improve comparision:
little representativeness of in-situ**

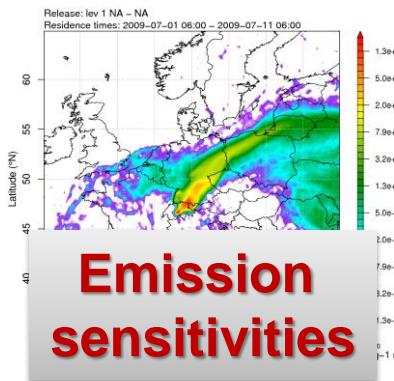
Conclusions

- WP5 mainly focussed on the development of a method to derive reference profiles from surface-in observations and independent model profiles
- Method offers a possibility to **quantitatively** validate remote sensing tropospheric products using surface in-situ observations
- It goes beyond a mere model to remote sensing comparison in that it incorporates dedicated transport simulations and an analysis of representativeness of the surface in-situ observation and transfers their information in the vertical (calibrating the model profile)
- Successfully applied to FTIR and MAXDOAS profile retrievals.
 - **Comparability enhanced** with in-situ profiles in contrast to in-situ only
 - increased correlation
 - decreased scatter
 - regression slopes close to unity for FTIR CO and O₃
 - reduced biases for all observations, but CH₄ at IZO
- Method reveals good ability of remote sensing techniques to detect **day-to-day variability**

LPDM Simulations

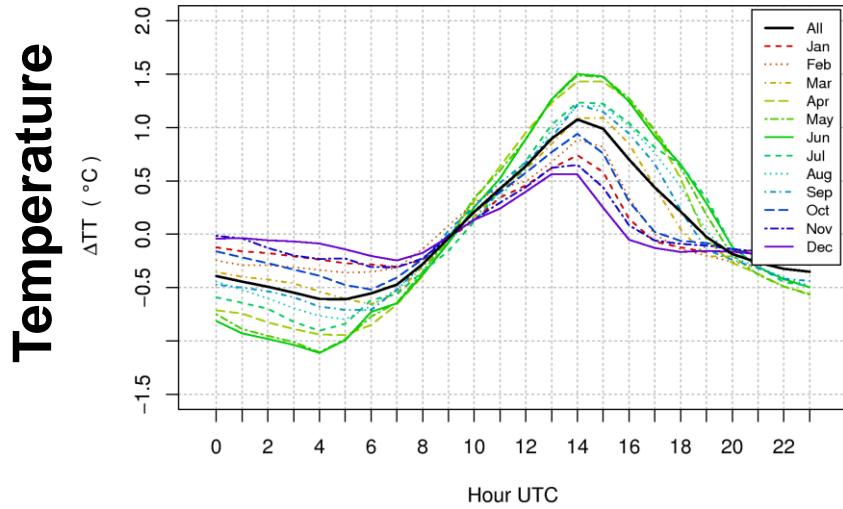
- Run **backward** Lagrangian Particle Dispersion (**LPDM**) calculations for all **different sampled air volumes**
- Derive recent (10 days) **emission influence**
- Simulate **mole fractions** for tracers (CH_4 , CO, O_3)
- Analysis of **representativeness** (comparison of recent influence) for filtering and in-situ extrapolation

C =

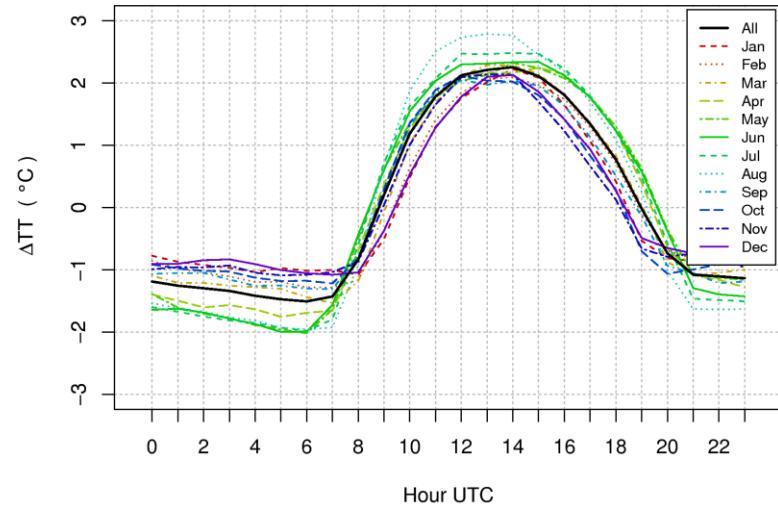


In-situ Diurnal Cycle

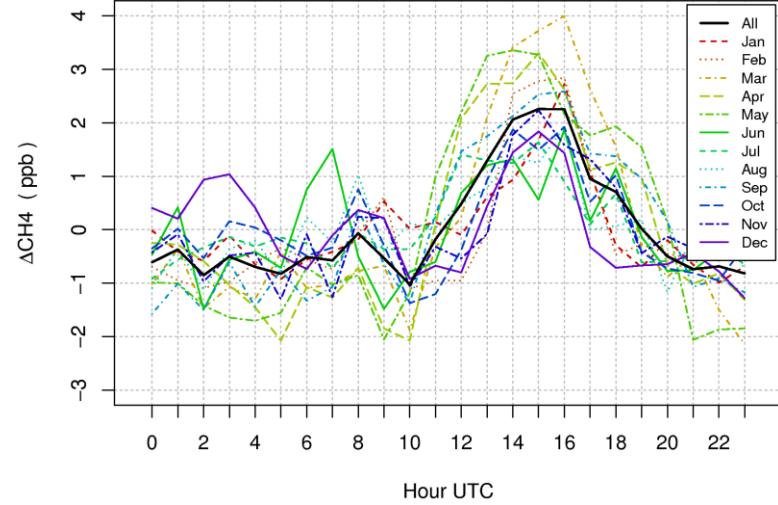
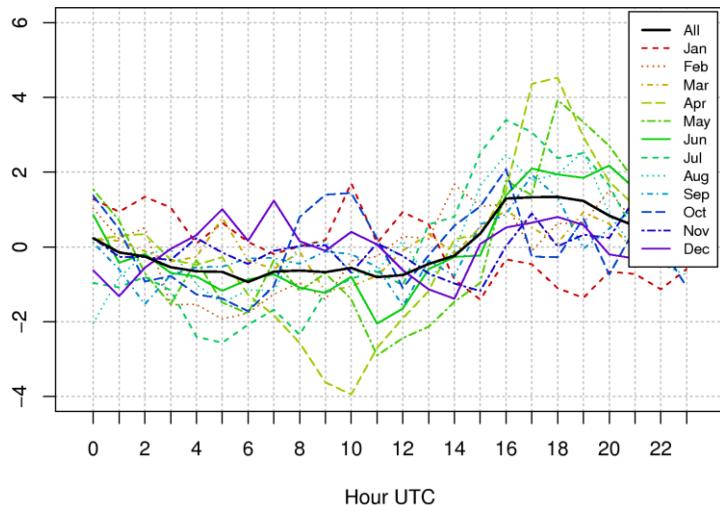
Jungfraujoch, 3580 m asl



Izaña, 2370 m asl



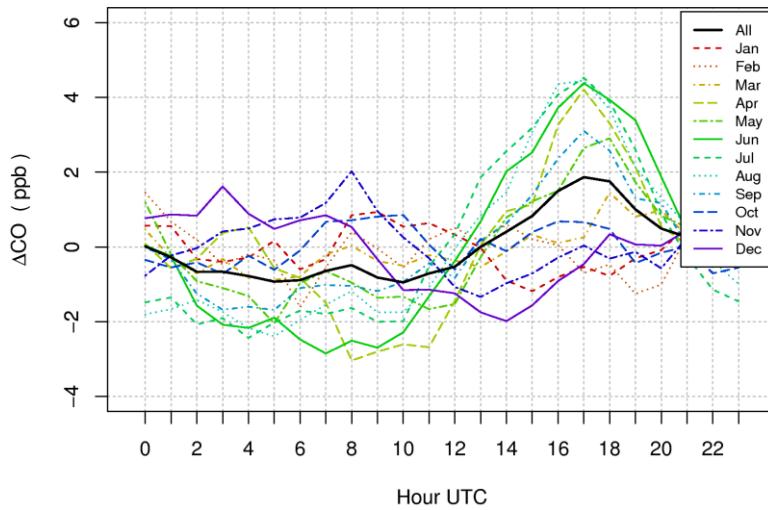
Methane



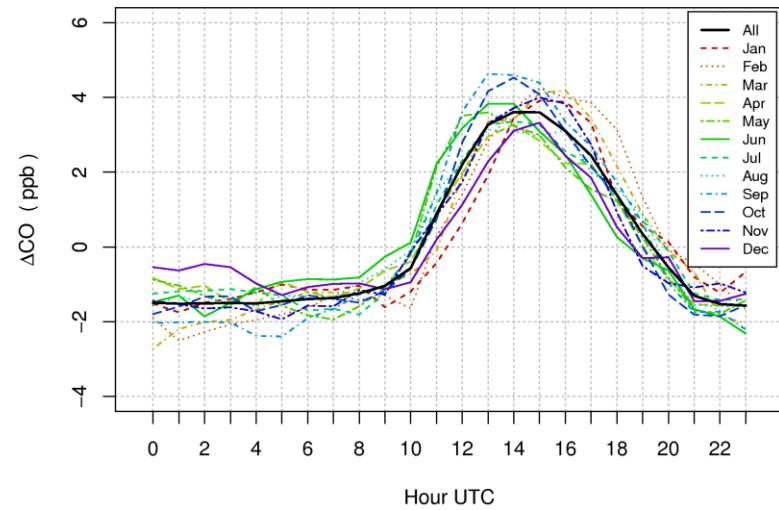
In-situ Diurnal Cycle

Carbon Monoxide

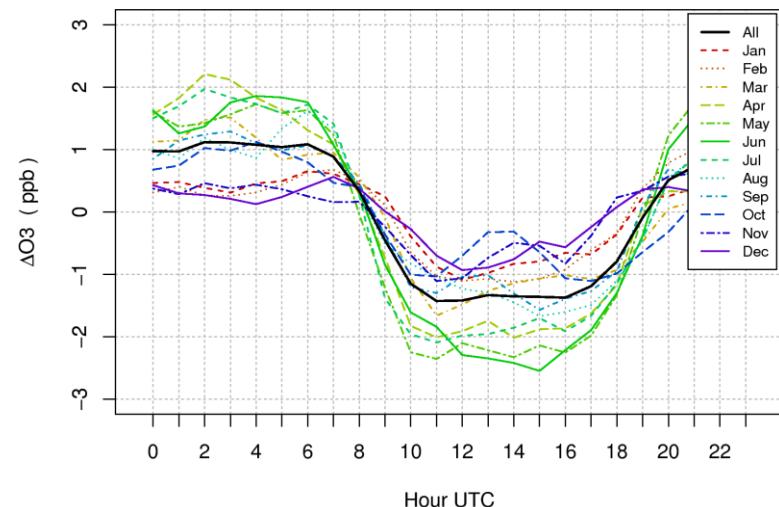
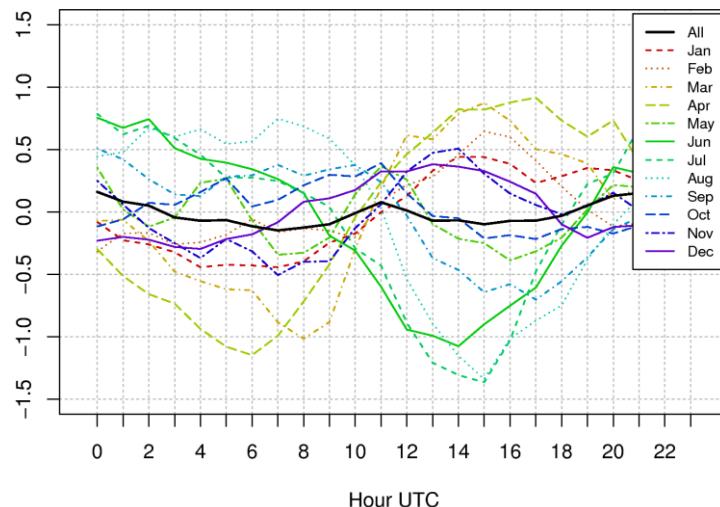
Jungfraujoch, 3580 m asl



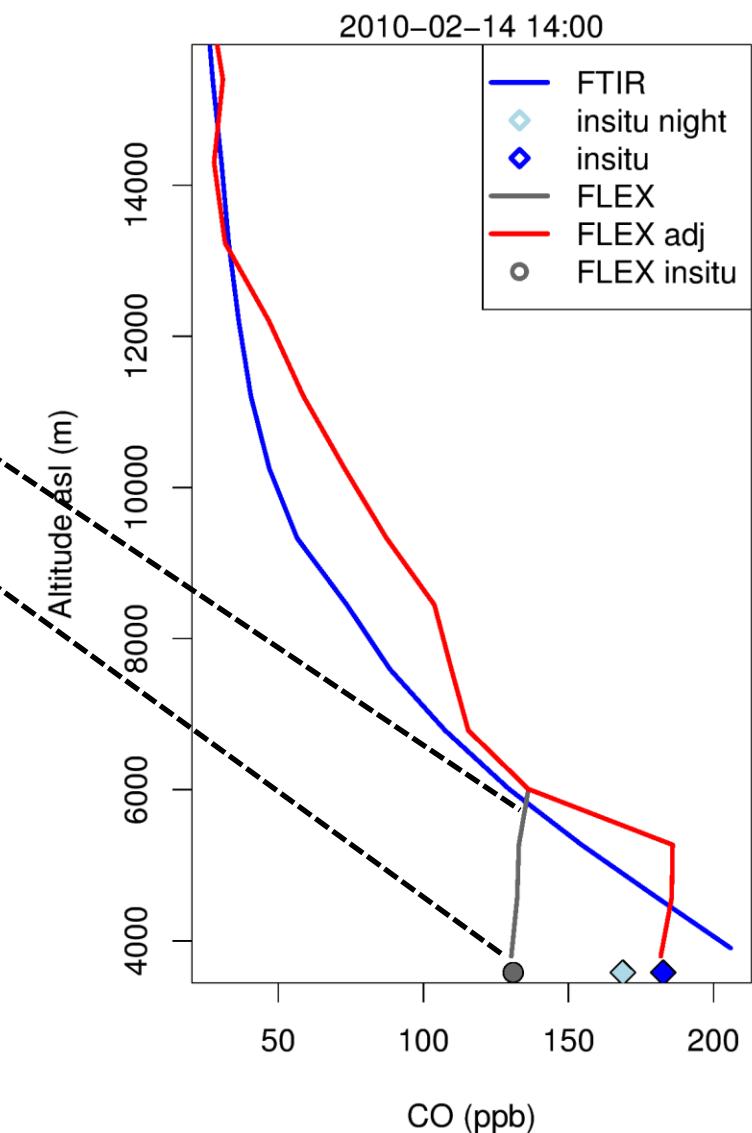
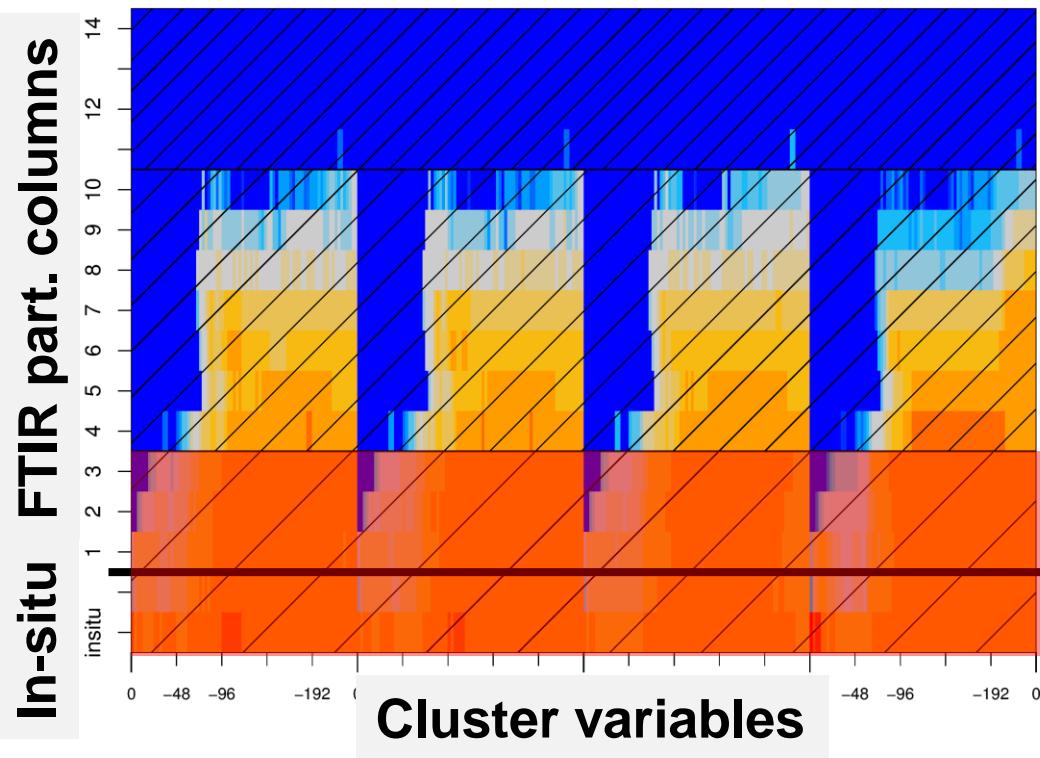
Izaña, 2370 m asl



Ozone



"In-situ Data Assimilation"



Adjustment of FLEPXART profile

- Separating background and pollution
- Bias correction for background
- Factorial correction for pollution