Co-ordinated by ECMWF

CoCO2
Prototype system for a Copernicus CO_2 service

WP4 LOCAL AND REGIONAL MODELLING AND DATA ASSIMILATION

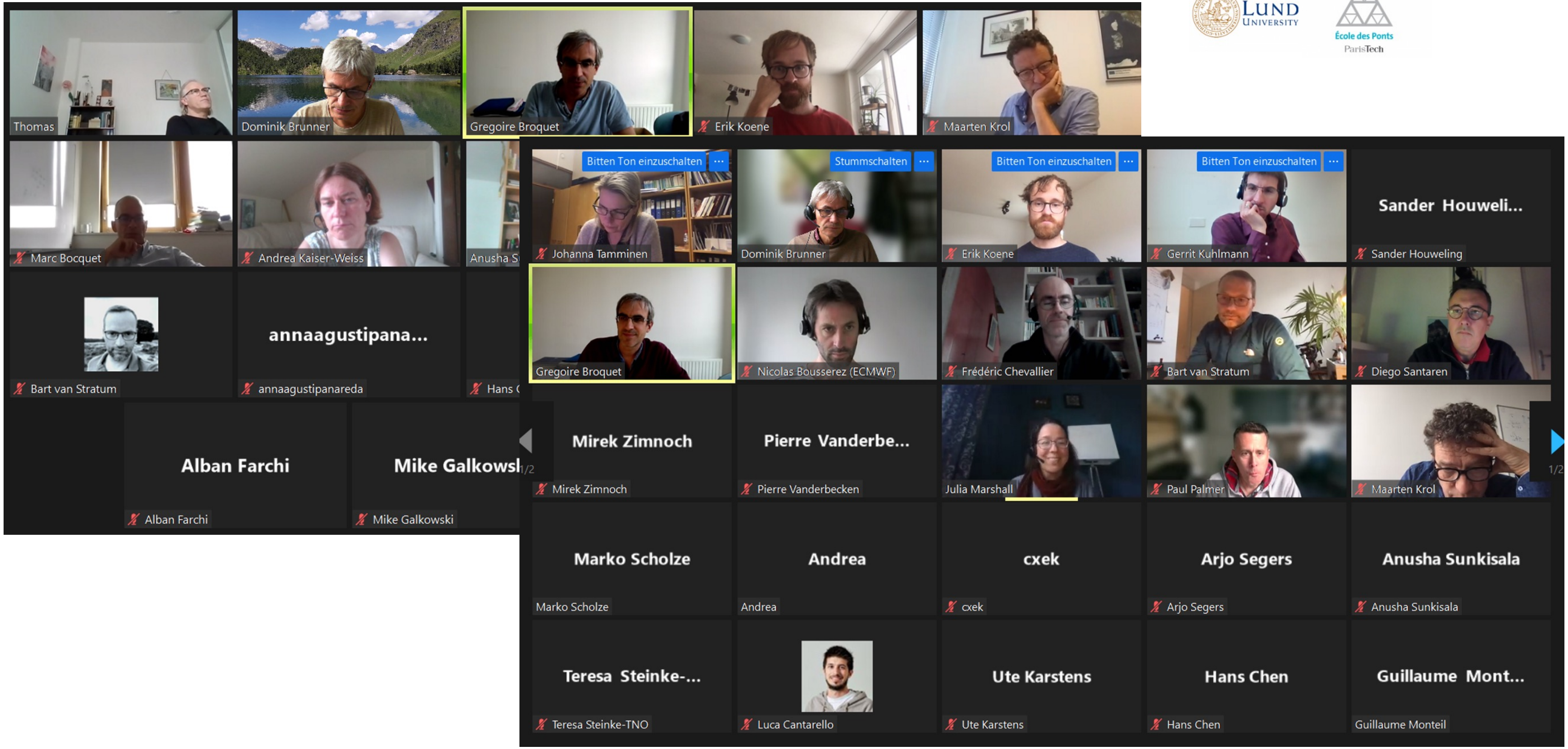
Grégoire Broquet, Dominik Brunner
and the WP4 team

CoCO2 Presentation Day

05/12/2022

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 958927.

WP4 - A large team effort



Overview WP4

Local scale – Point sources and Cities

T4.1 Local scale model performance assessment and improvement
EMPA, *WU, CEA,VUA, MPG, FMI, TNO, DWD, ENPC, ECMWF*

T4.2 Local inversion approaches for efficient processing of plume images with a large spatial and temporal coverage
FMI, *CEA, EMPA*

T4.3 Local inversion approaches using atmospheric transport models
ENPC, *CEA, iLab, WU, UEDIN, FMI, VUA, AGH*

National scale

T4.4 National scale inversions
DLR, UEDIN, *TNO, DWD, EMPA, CEA, ENPC, VUA, FMI, ULUND, ECMWF, AGH*

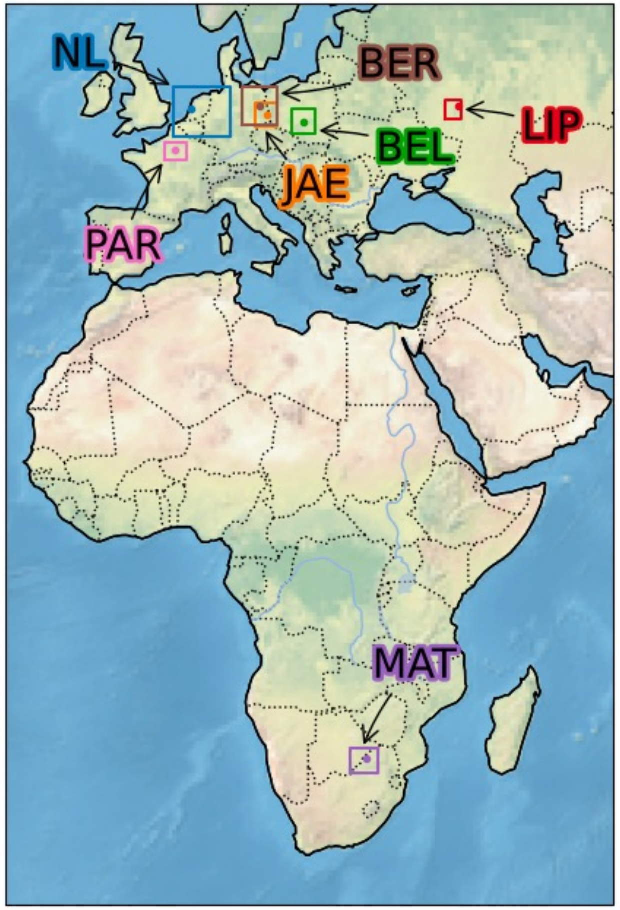
T4.5 Guidance and synthesis between the local and regional scale estimates
CEA *+ all*

Task 4.1. Local scale models: performance assessment & improvement

D4.2: Assessment of plume model performance, due Dec 2022

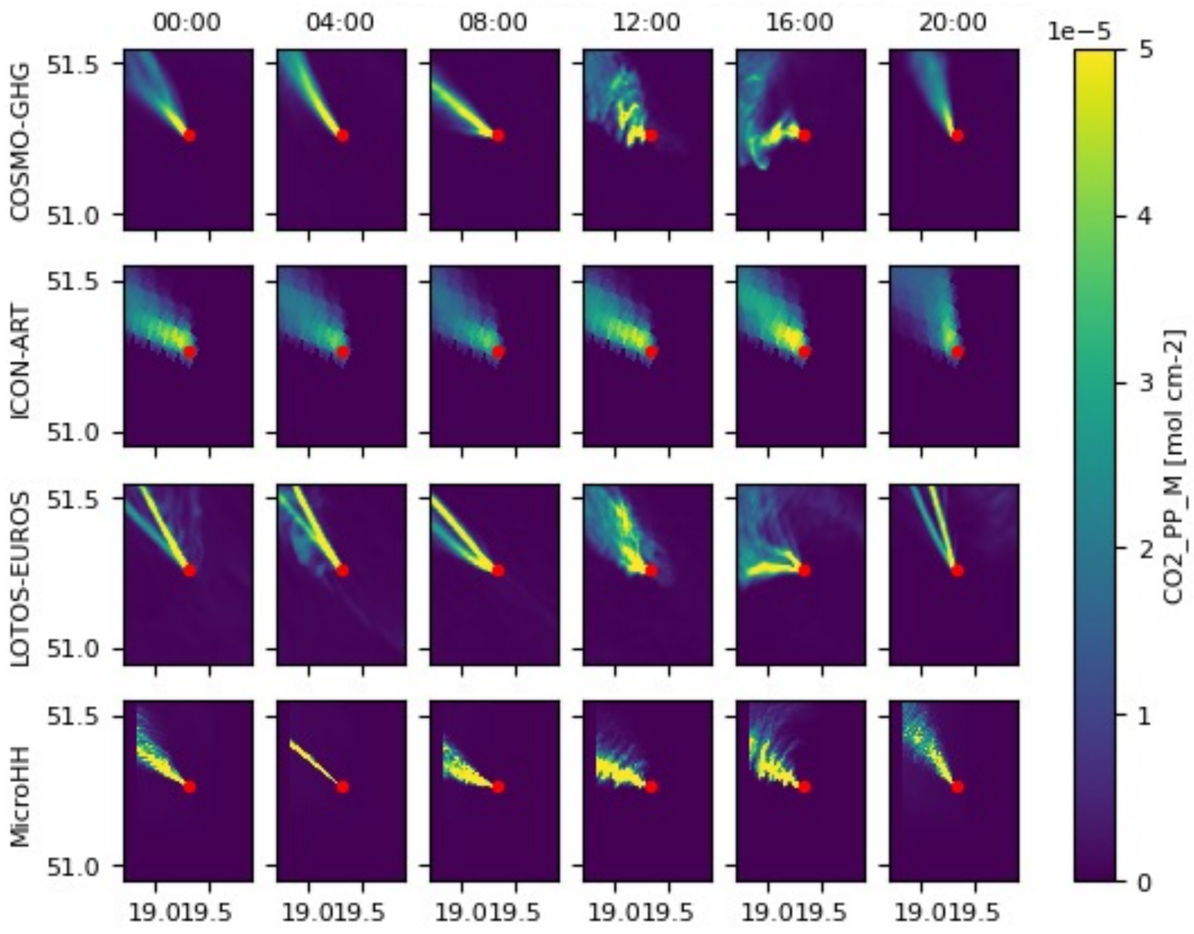
Overview of plume simulations

ID	Description	Time period	Available observations	Modeled with
BEL	**Power plant** Bełchatów, Poland	6-7 Jun 2018	In-situ observations (CO_2) and remotely sensed observations (XCO_2) from three aircraft; TROPOMI NO_2	COSMO-GHG, ICON-ART, LOTOS-EUROS, MicroHH
JAE	**Power plant** Jänschwalde, Germany	22-23 May 2018	In-situ observations (CO_2) and remotely sensed observations (XCO_2) from two aircraft; TROPOMI NO_2	COSMO-GHG, ICON-ART, LOTOS-EUROS, MicroHH
LIP	**Steel plant** Lipetsk, Russia	12-13 Jun 2019	TROPOMI CO	COSMO-GHG, MicroHH
MAT	**Power plant** Matimba, South Africa	24-25 Jul 2020	TROPOMI NO_2	COSMO-GHG, MicroHH
BER	**Berlin** urban area, Germany	18-27 Jul 2018	In-situ observations (CO_2) from one aircraft; TROPOMI NO_2.	COSMO-GHG, LOTOS-EUROS
PAR	**Paris** urban area, France	1-8 Aug 2018	Seven high-precision stationary CO_2 measuring stations; TROPOMI NO_2	COSMO-GHG, WRF-CHEM
NL	**Randstad** area Netherlands	16-23 Jun 2018 16-23 Dec 2018	One high-precision stationary CO_2 measuring station; 43 stationary NO_2 measuring stations; TROPOMI NO_2	LOTOS-EUROS



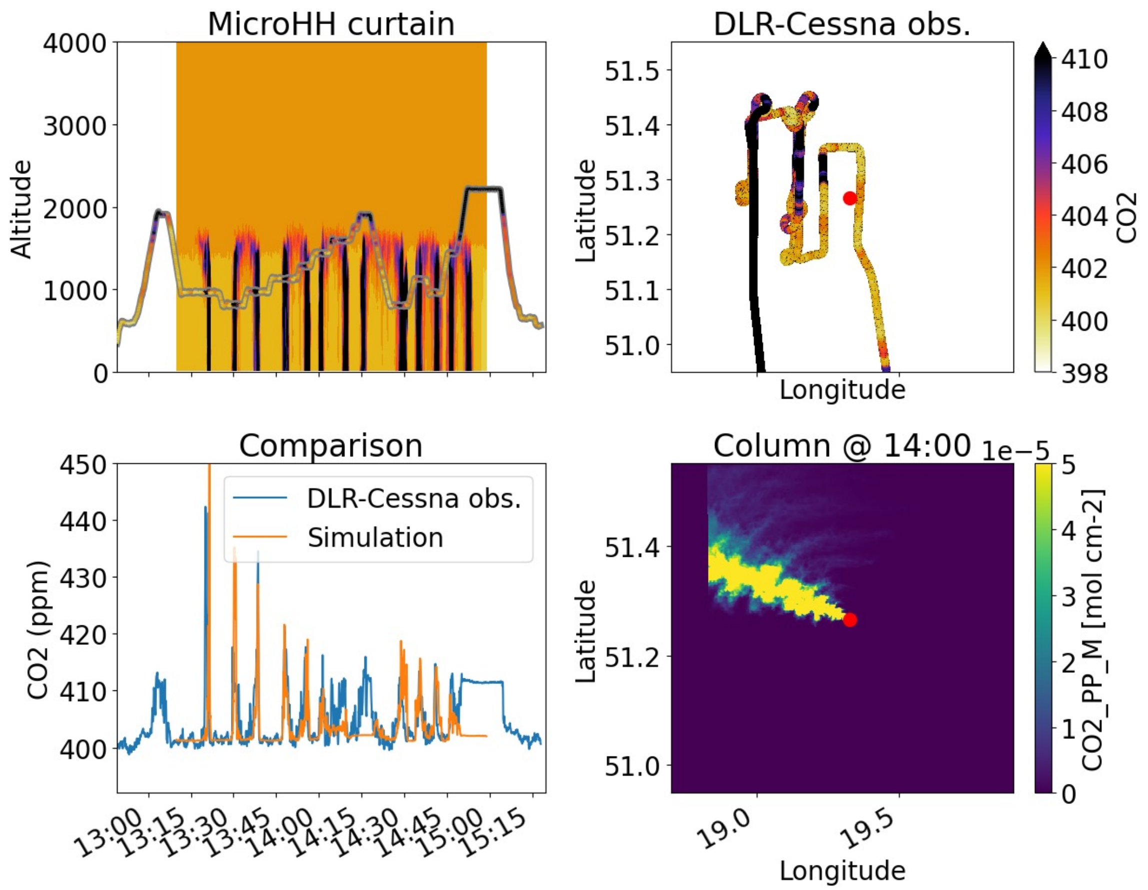
Example 1: Power plant Belchatow, Poland, 7 Jun 2018

Column XCO_2 at different day times



Comparison with aircraft in-situ CO_2

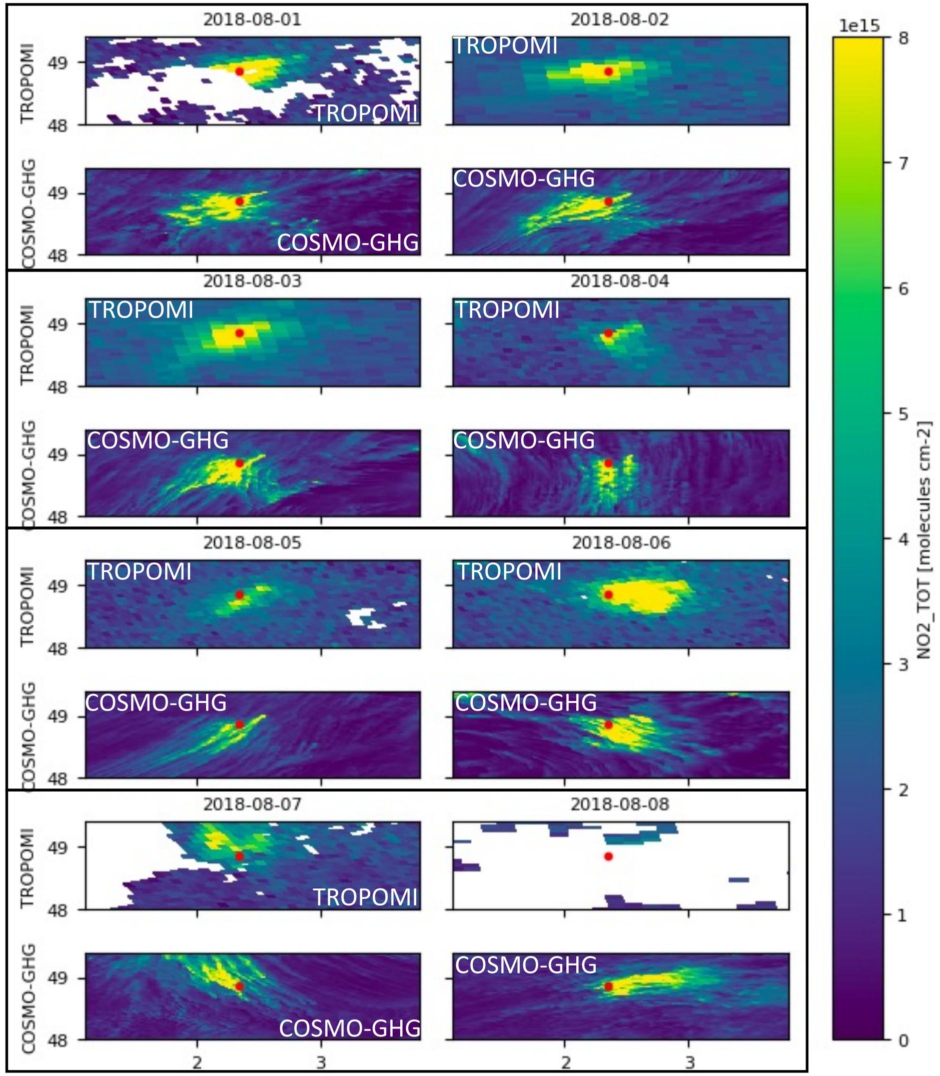
(COMET campaign, courtesy DLR)



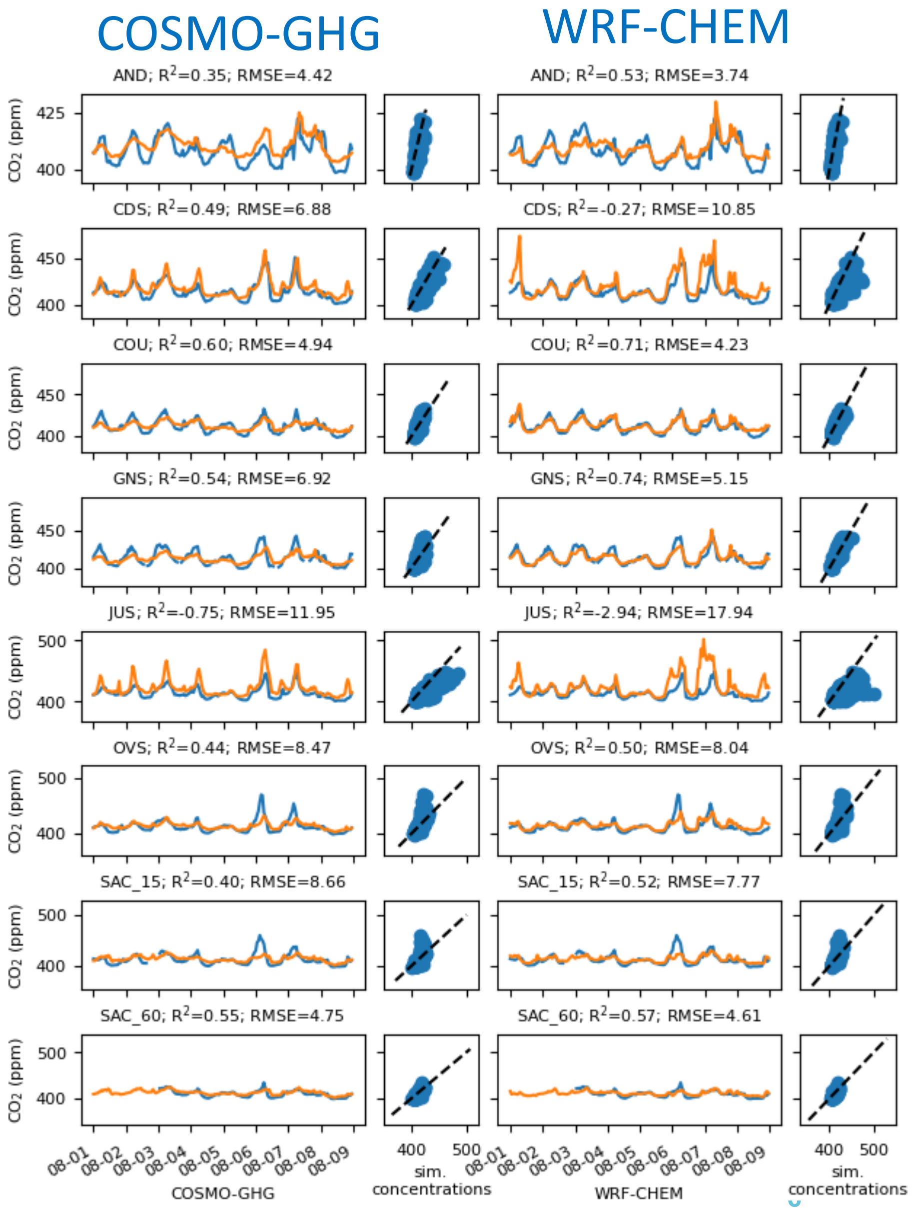
Task 4.1. Local scale models: performance assessment & improvement

Example 2: City of Paris, 1-10 Aug 2018

TROPOMI
NO_2
1-8 Aug



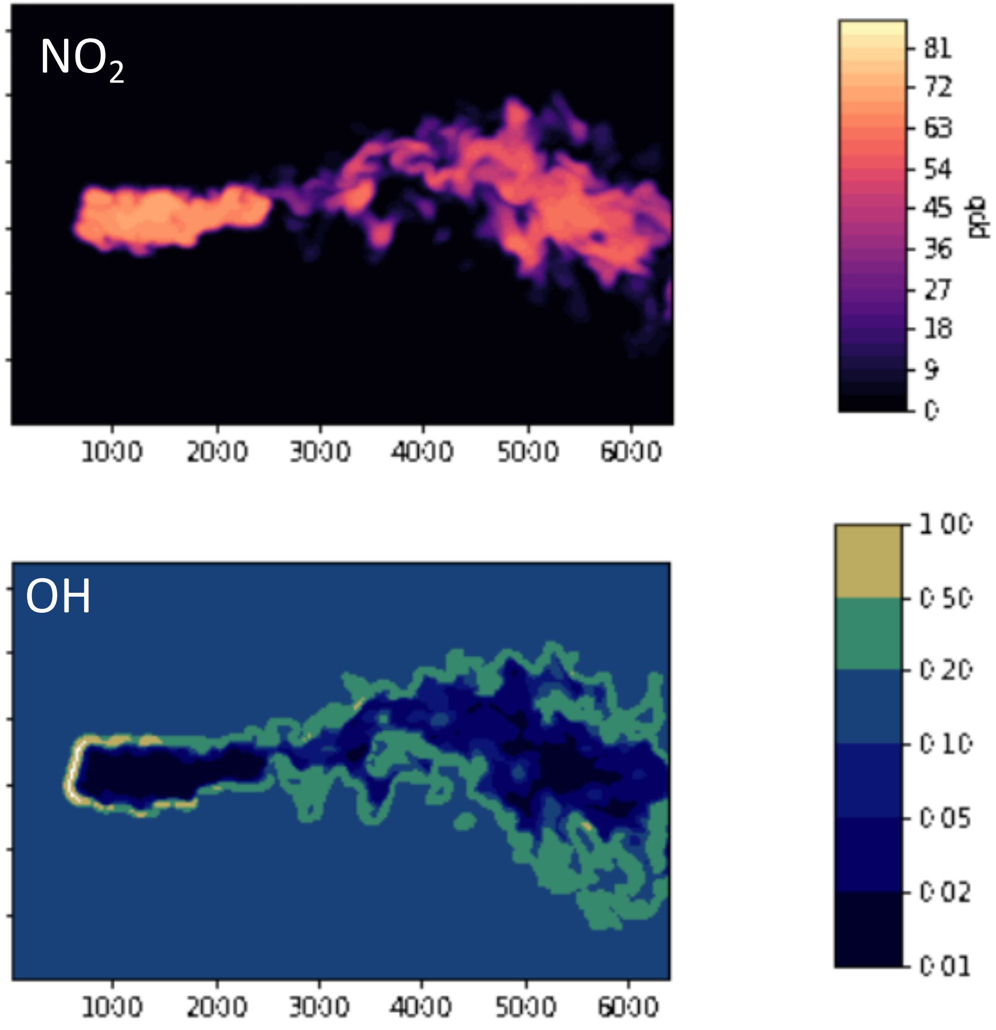
tower
in-situ
CO_2
1-9 Aug



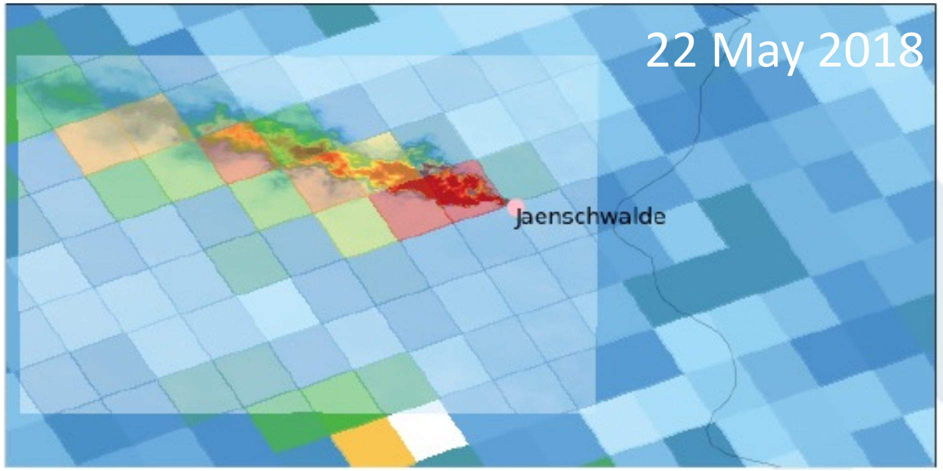
Task 4.1. Local scale models: performance assessment & improvement

Simplified chemistry simulations with MicroHH (M. Krol, WUR)

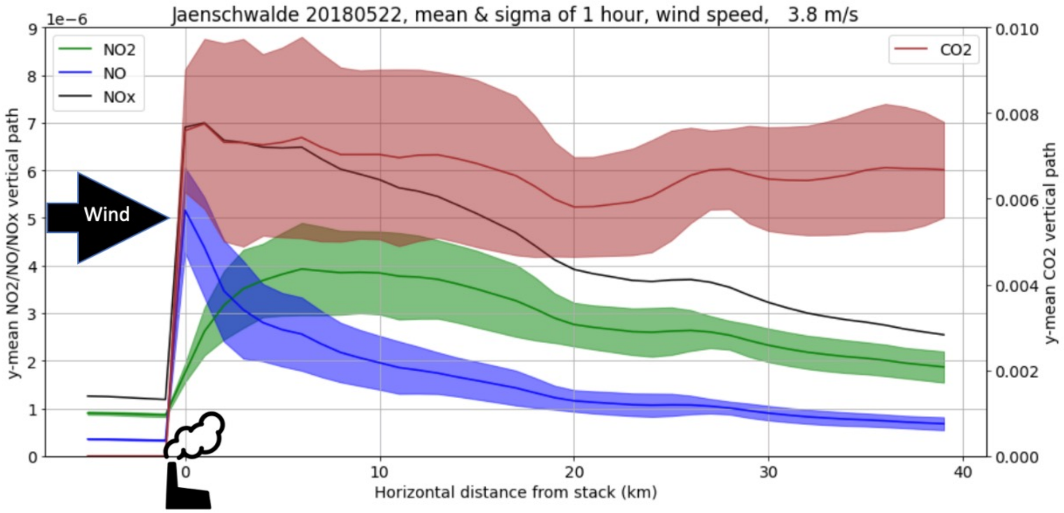
Snapshot of simulation at 25 m resolution



Comparison with TROPOMI



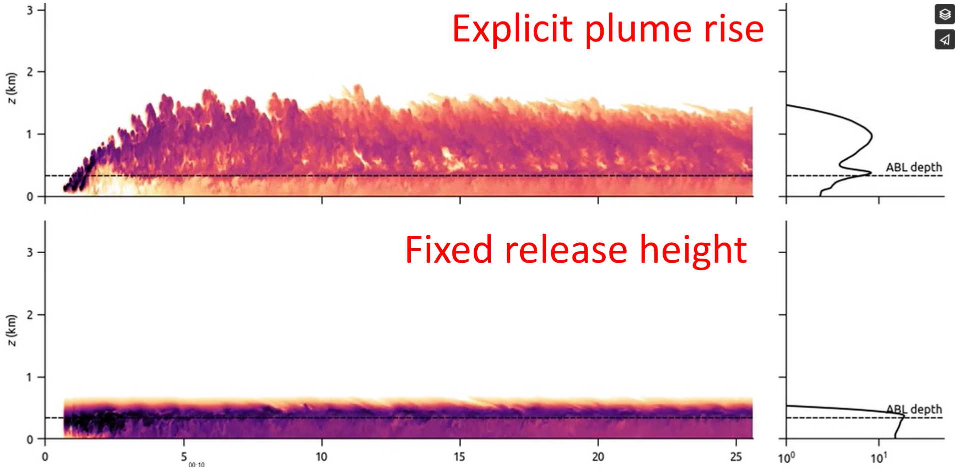
NO, NO$_2$, NO$_x$ and CO$_2$ along plume



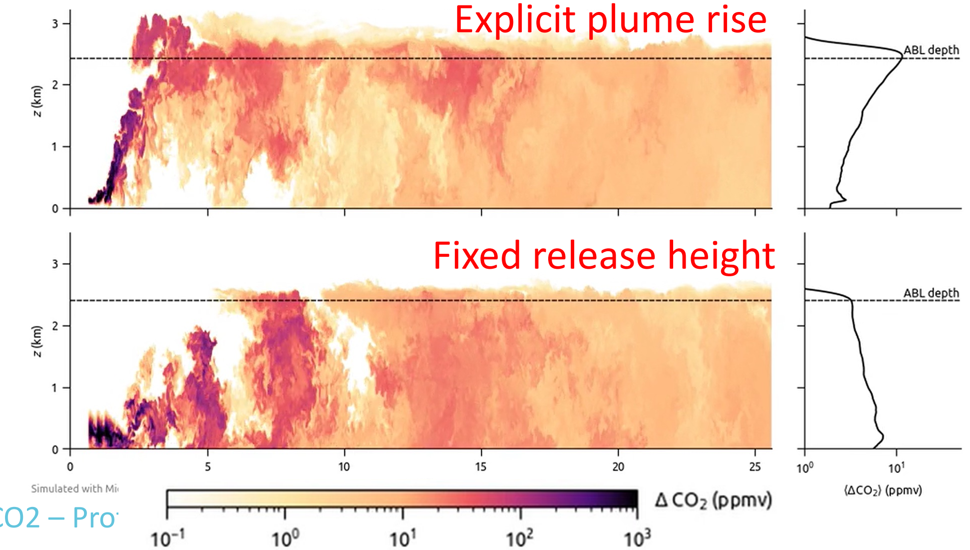
Task 4.1. Local scale models: performance assessment & improvement

Plume rise simulations for Jänschwalde with MicroHH (B. van Stratum, WUR)

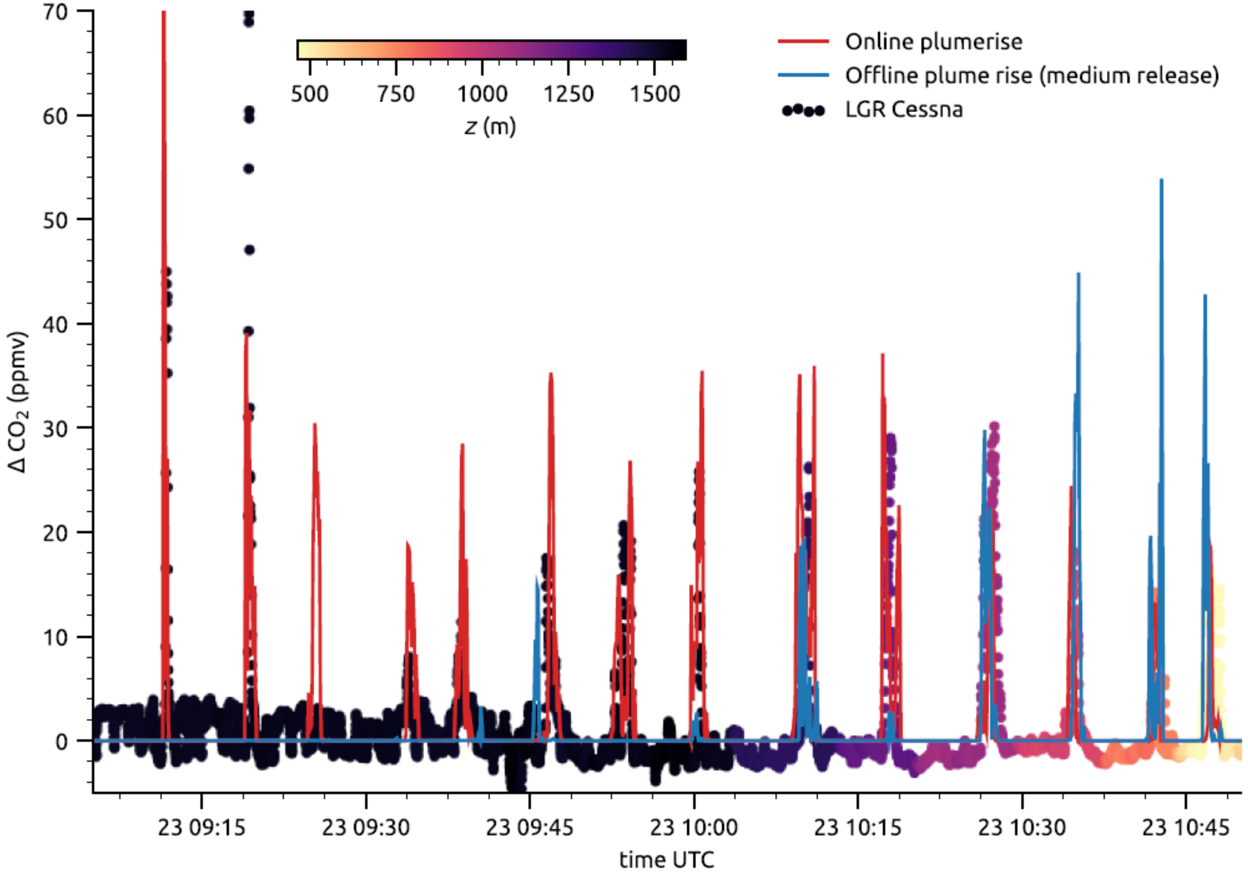
Early morning 06:00



CO2M overpass time 11:30



Comparison with aircraft in-situ CO_2 observations



https://vimeo.com/channels/microhh/768081104

Task 4.2: Light plume detection & quantification methods

D4.4: Benchmarking of plume detection and quantification methods, due Dec 2022

Methods tested

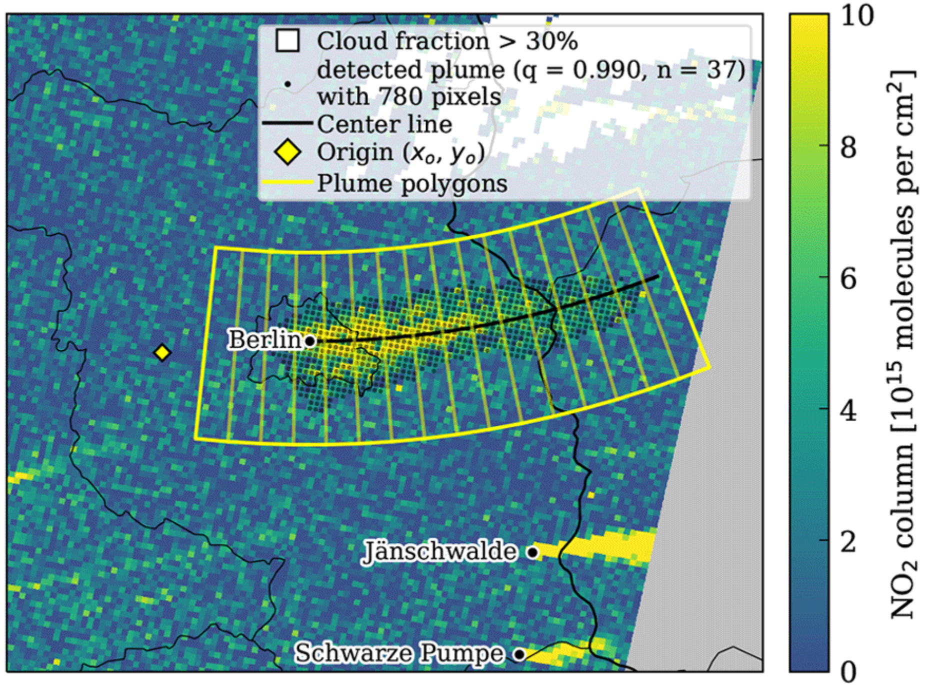
- EMPA: Cross Sectional (CS)
- EMPA: Gaussian Plume (GP)
- EMPA: Integrated Mass Enhancement (IME)
- LSCE: Light Cross Sectional (LCS)
- FMI: Divergence (DIV)

Benchmarking data and configurations

- Synthetic CO2M observations of XCO_2 and NO_2 from SMARTCARB
- 2 periods: full year 2015, 3 months May - Jul
- 2 cloud conditions: With and without
- 2 auxiliary tracer cases: With and without NO_2
- 2 wind fields: COSMO and ERA5 winds

Further tests with real TROPOMI observations and simulated plumes from Task 4.1

Example of plume detection



Technical details

- All methods implemented in *python package ddeq* *https://gitlab.com/empa503/remote-sensing/ddeq*
- Data on *ICOS fileshare* https://fileshare.icos-cp.eu
- Analysis with *jupyter notebooks at ICOS-CP*

Task 4.2: Light plume detection & quantification methods

Beirle's divergence method applied to XCO2 observations

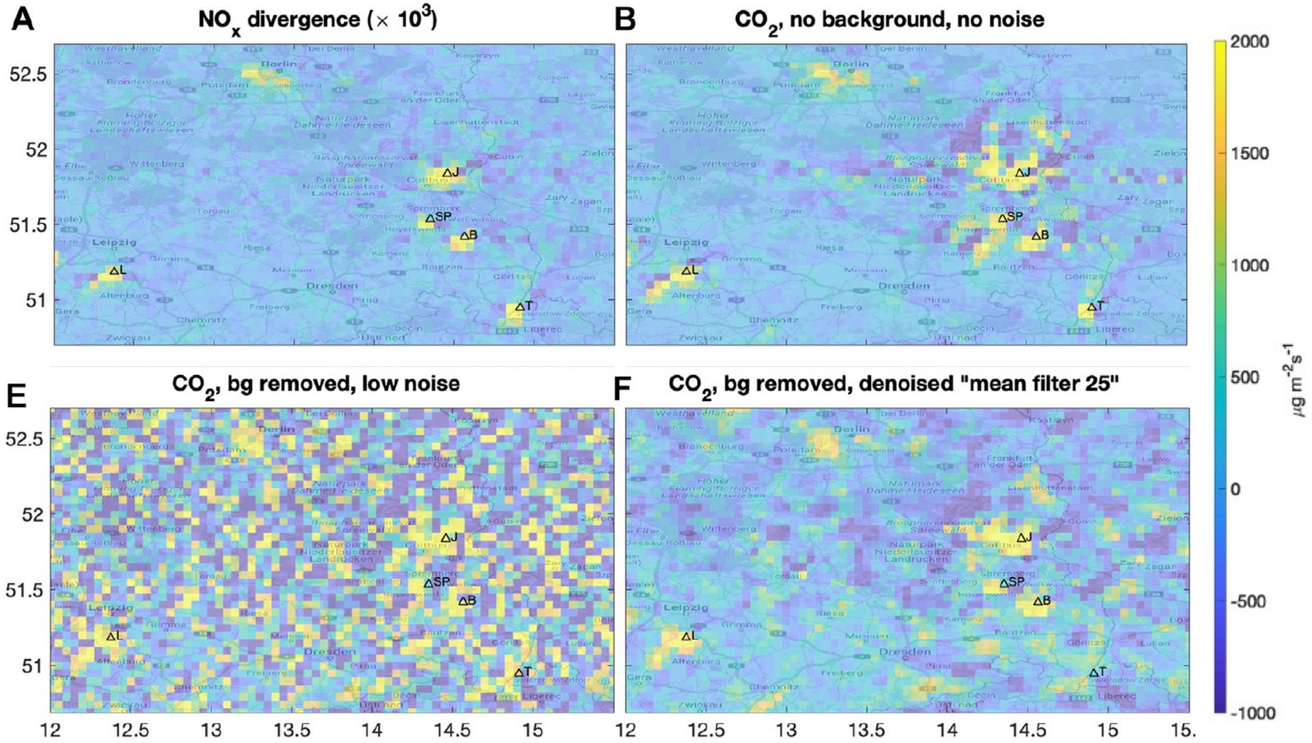
(Hakkarainen et al., Frontiers in Remote Sensing, 2022)

Flux divergence equals sum of emissions *E* and sinks *S:*

$$\nabla \cdot F = E - S \qquad F = (F_x, F_y) = (V \cdot u, V \cdot v)$$

V = vertical column density from satellite
u, v = horizontal wind components, e.g. from ERA5

Divergence maps for NO_x and CO_2



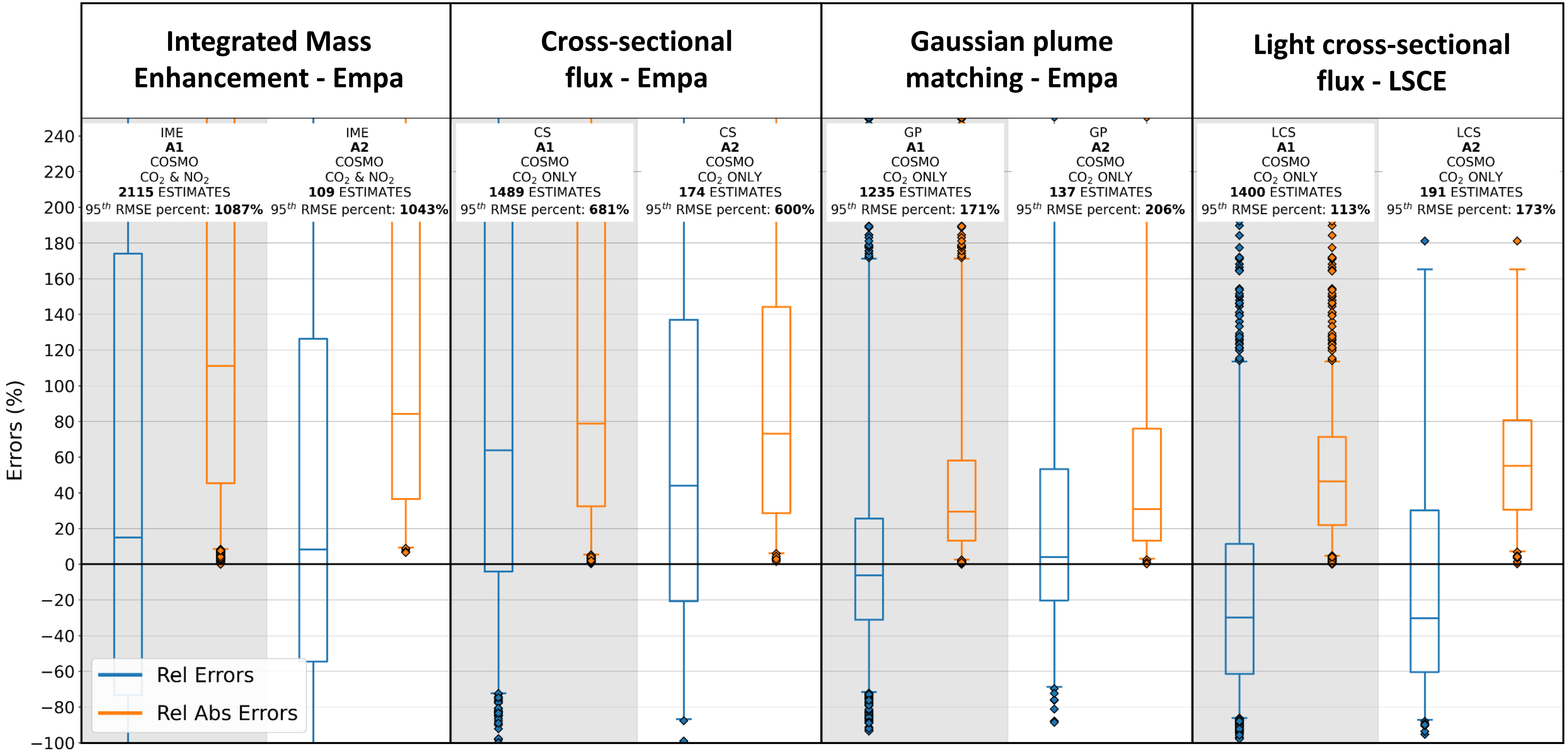
Method works well for NO_x

Additional challenges for CO_2:

- Much lower signal:noise, denoising necessary
- High background levels need to be subtracted before applying method
- Biospheric fluxes
- Strict cloud filtering needed

Task 4.2: Light plume detection & quantification methods

Impact of clouds: Compare benchmark results btw. cases A1 (no clouds) and A2 (cloud threshold)

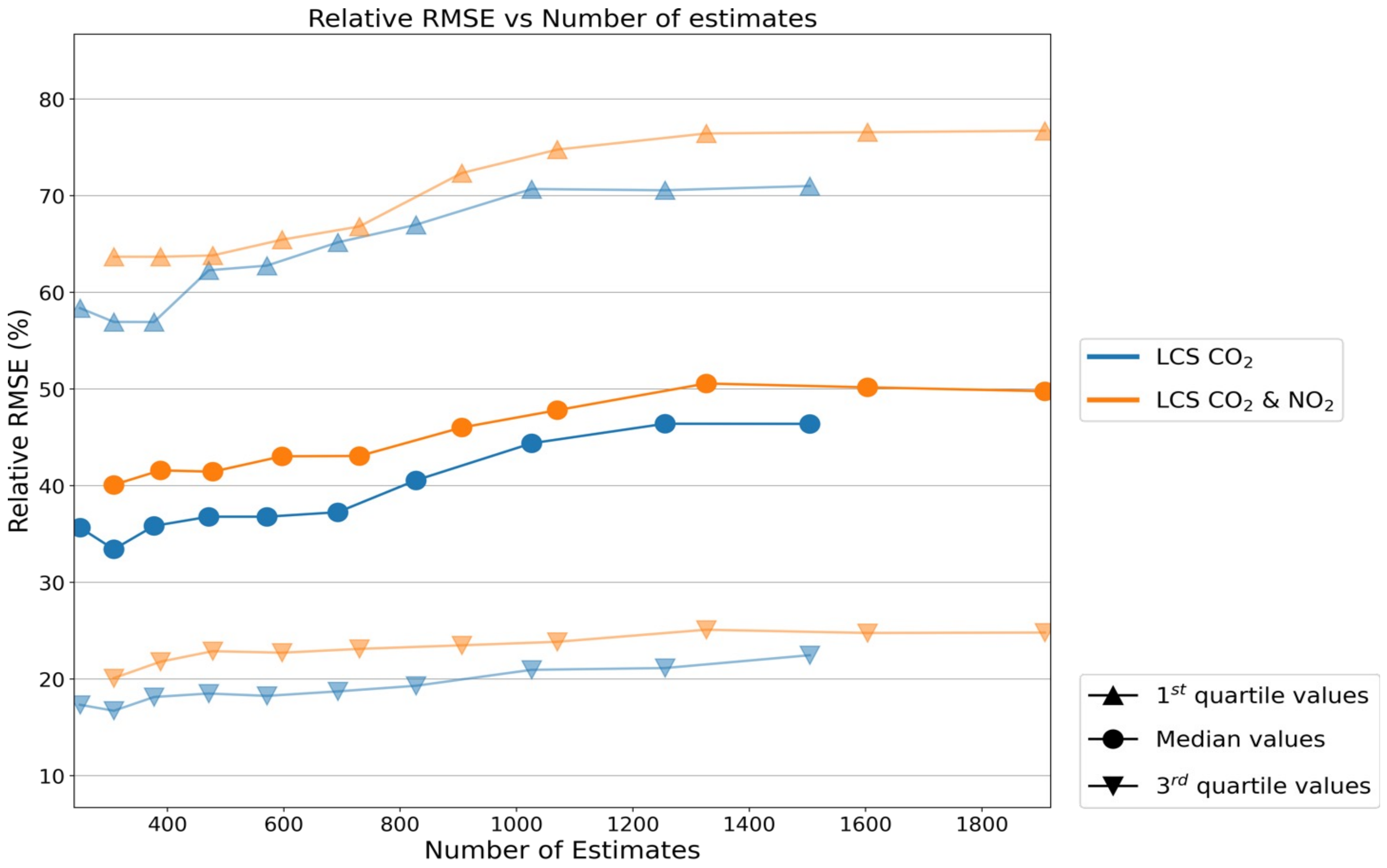


Task 4.2: Light plume detection & quantification methods

Impact of quality filtering for poor plume detection & quantification cases

-> Tradeoff between number of estimates and quality of results

Results from light cross-sectional flux method of LSCE for case A1 (no clouds)



less strict quality filtering

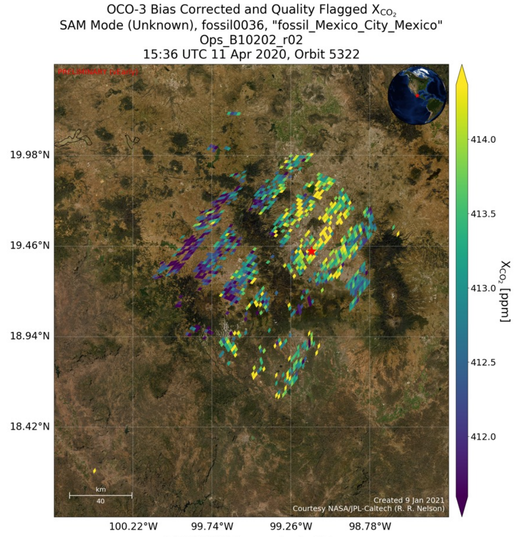
Task 4.3: Local inversions using atmospheric transport models

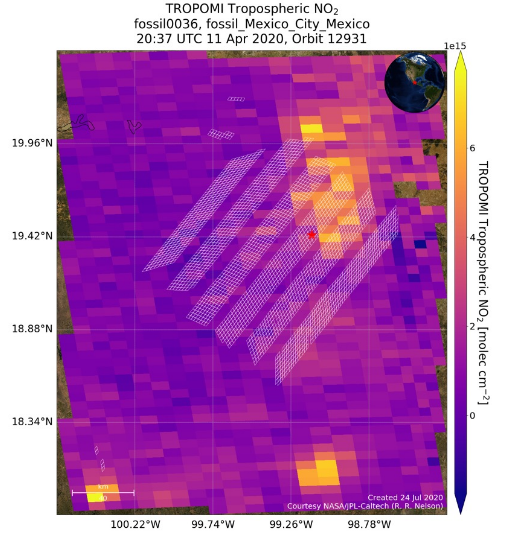
- **Objective**: develop approaches using info from high resolution models to detect & invert plumes in XCO2 images
- **estimates of the sources (industrial sites, cities) in complex situations** where the light approaches (T4.2) face limitations

→ **insights on spatial & sectoral distribution of emissions in cities**

T4.3.1 **Overcoming uncertainties in transport model**	New metrics for comp of model vs observed plume	Tests on pseudo images of XCO2 plumes from Paris, Berlin and power plants	CEREA
	Using CNN trained on model to detect & invert plumes		
Potential of the co-assimilation of CO or NO2 images for cities	Analysing CO/CO2 & NO2/CO2 ratios over urban areas	Global analysis of TROPOMI NO2/CO & OCO-2/3 XCO2	UEdin
Inferring spatial & sectoral distribution of city emissions **Optimizing city-scale inversion configurations** **Assessing their robustness**	Propagation of uncertainties with a HR DA system	CCFFDAS assimilating XCO2 and NO2 images over Berlin	iLab
	Tests with pseudo images from LES model	EnKF over the Randstad area	VUA
T4.3.2	Tests with real measurements	Analytical inv. over Krakow	AGH

Snapshot Area Map (SAM) of XCO_2 over Mexico by OCO-3 and comparison to TROPOMI NO_2 (source: JPL)





Non local evaluation metrics to compare modelled and observed plumes which does not penalize isometries

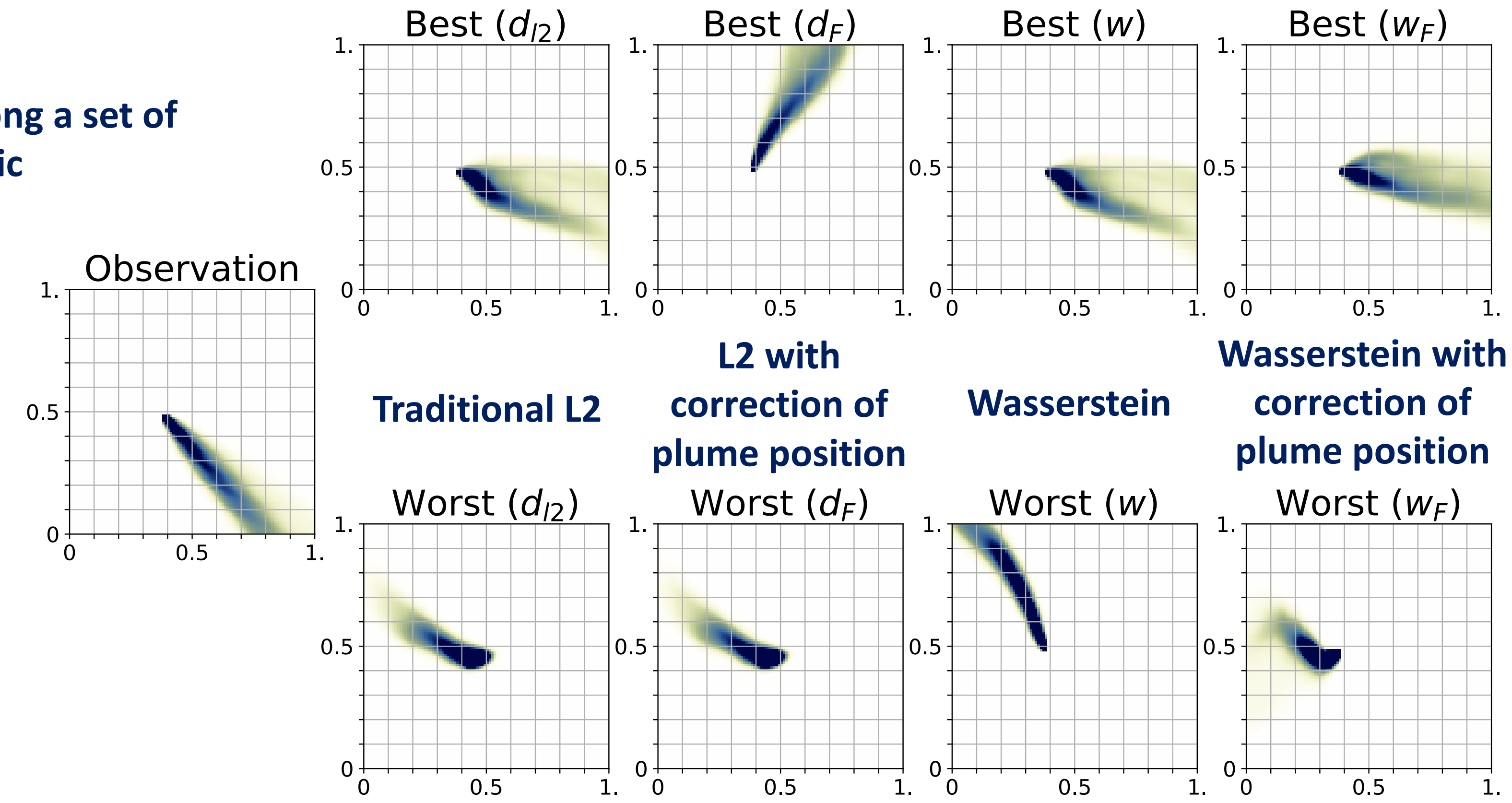
Vanderbecken et al., 2022, AMTD

Testing four metrics

Best and worst fit to observed plumes among a set of modelled plumes as a function of the metric

Test on simulations from E. Potier (LSCE)

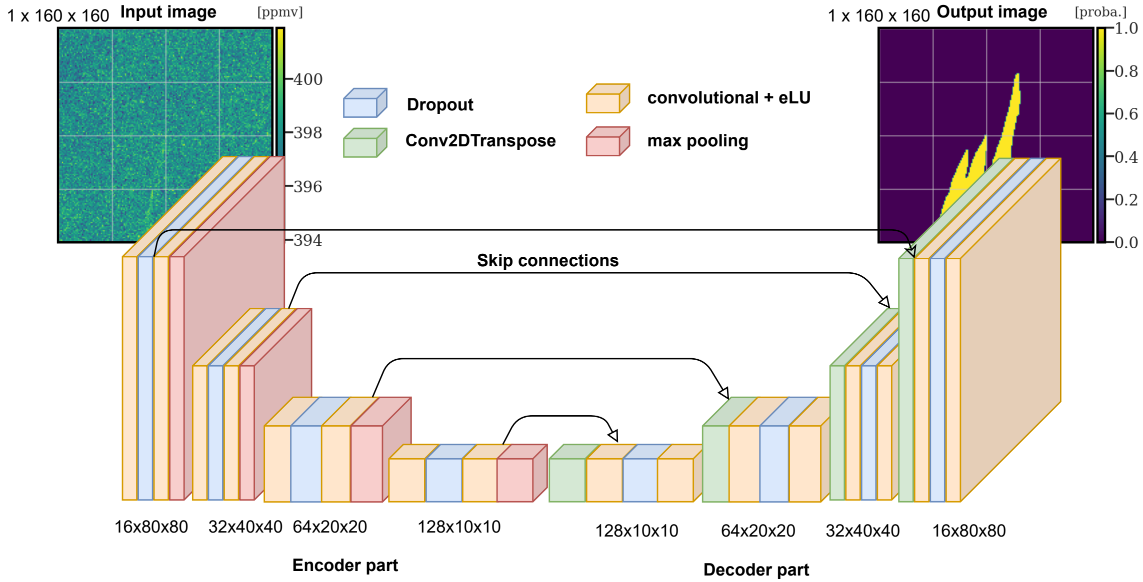
- **Baseline $\mathscr{L}_2$ metric (d_{l2}):**
  - (+) Easy to compute.
  - (-) double penality issue.
- **New local metric (d_F) freed from position error:**
  - (+) Keep $\mathscr{L}_2$ formalism while addressing double penalty issue.
  - (-) Add a local minimisation process.
- **Non-local Wasserstein metric (w):**
  - (+) Separation of the errors sources.
  - (-) Loose of the scale information.
- **Non-local Hellinger metric (w_F):**
  - (+) Cheap and freed of position error.
  - (-) Ground on Gaussian puff assumption.



Subtask 4.3.1: New inversion methods

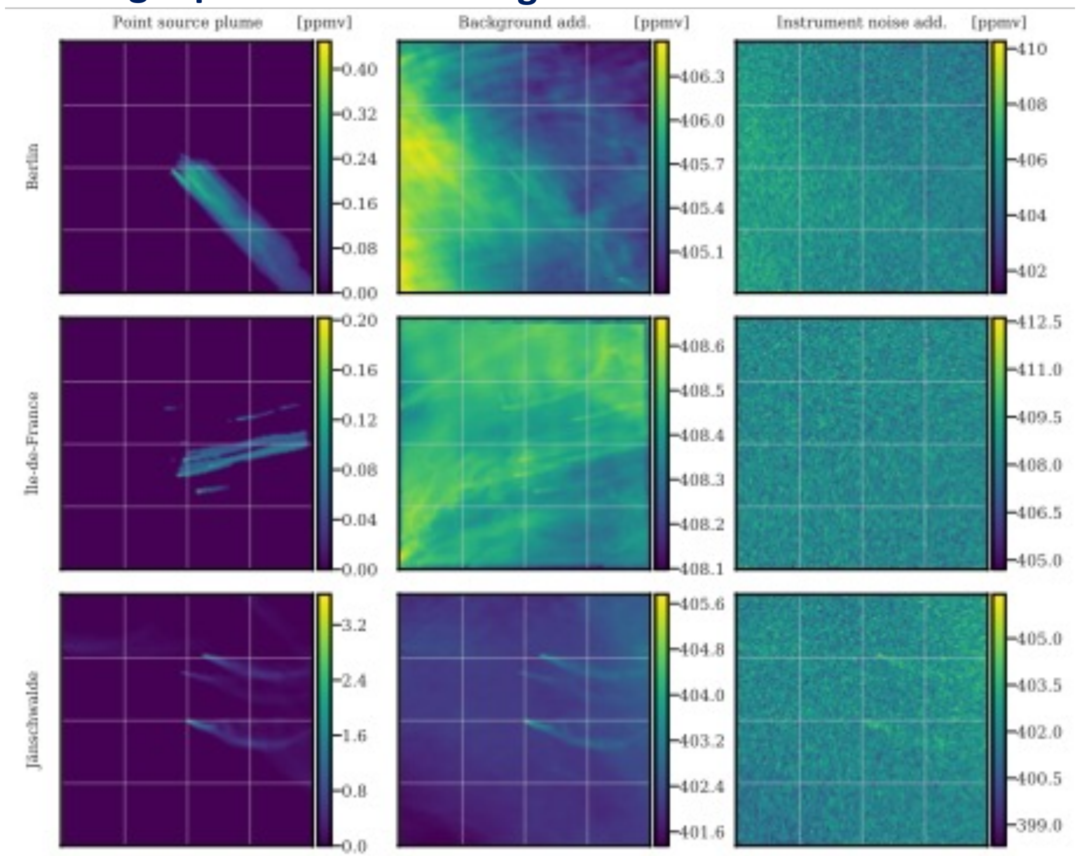
Plume segmentation and inversions based on Convolutional Neural Networks

J. Dumont Le Brazidec / CEREA



Plume segmentation: U-Net algorithm fed with pairs of XCO2 full fields and plume mask

Examples of XCO2 field simulation



- **Tests on XCO2 pseudo-images**
  - → modeled with WRF-Chem around Paris (LSCE/Suez Origins)
  - → modeled with COSMO-GHG around Berlin & Power Plants in Germany (SMARTCARB project / EMPA)

Subtask 4.3.1: New inversion methods

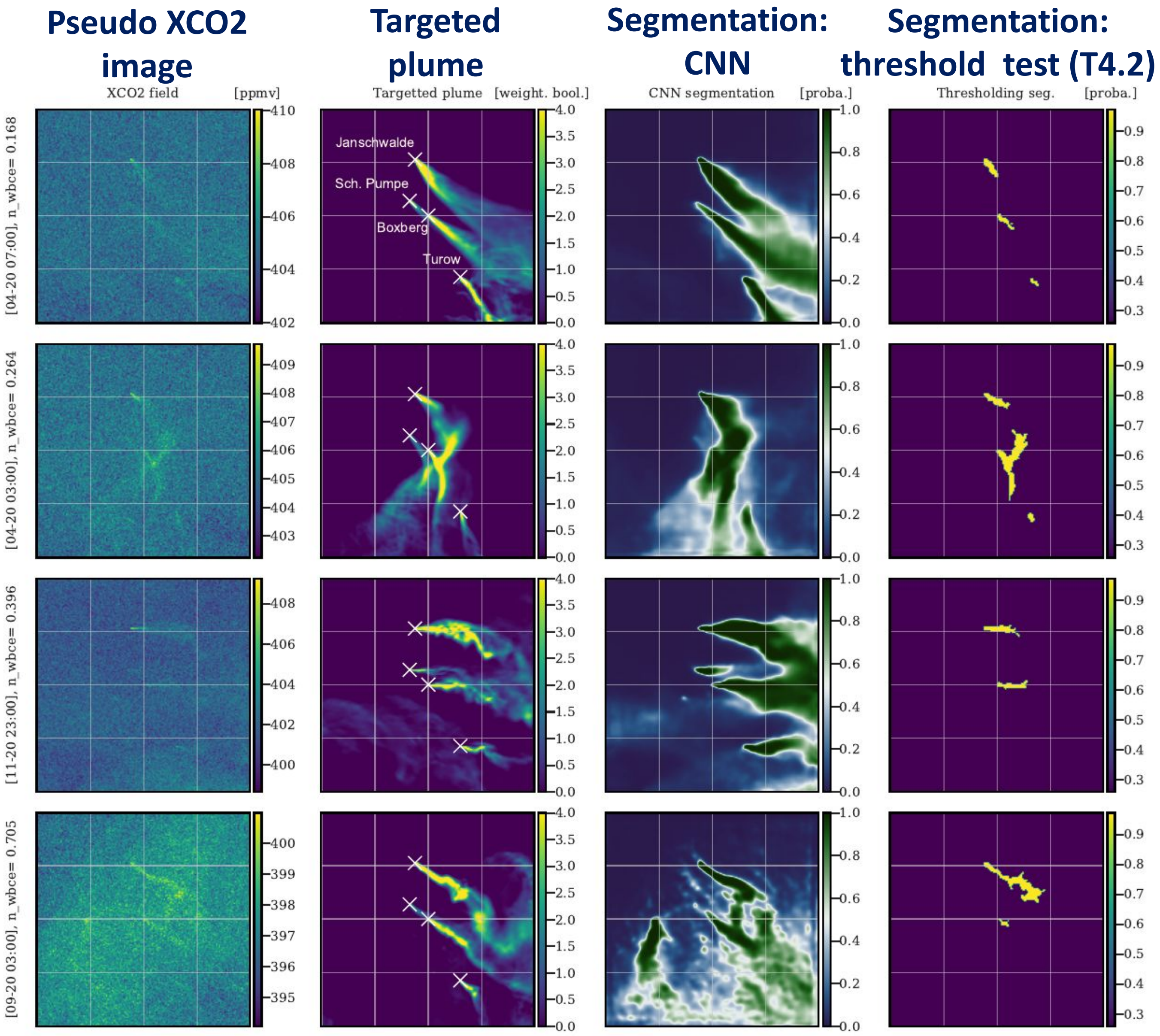
Plume segmentation based on Convolutional Neural Networks

Dumont Le Brazidec et al., 2022, submitted to GMD

Training and tests on images of the cluster of PP plumes around Boxberg

Rows = quartiles of performances from best to worst: the performance is based on a weighting of the plume mask by the plume concentration

→ Ability to handle overlapping plumes



Subtask 4.3.1: New inversion methods

Plume segmentation based on Convolutional Neural Networks

Dumont Le Brazidec et al., 2022, submitted to GMD

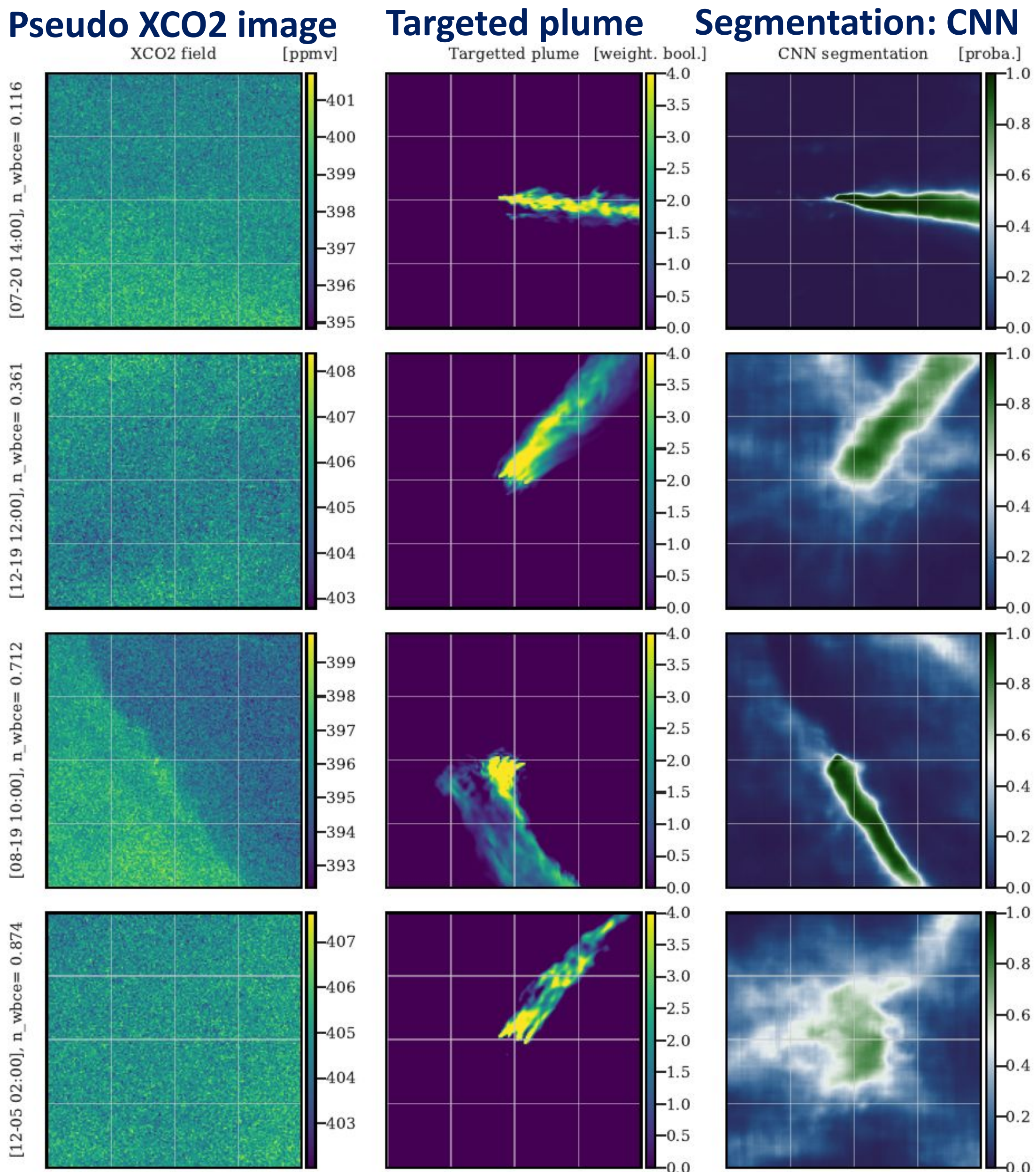
Training on images over Paris + PP and tests on images of the plume from Berlin

Rows = quartiles of performances from best to worst: the performance is based on a weighting of the plume mask by the plume concentration

- performances close to those when training the CNN with images from Berlin

→ **towards a “universal” algorithm** trained with a limited set of simulations to cover wide sets of sources: **from high to low cost method**

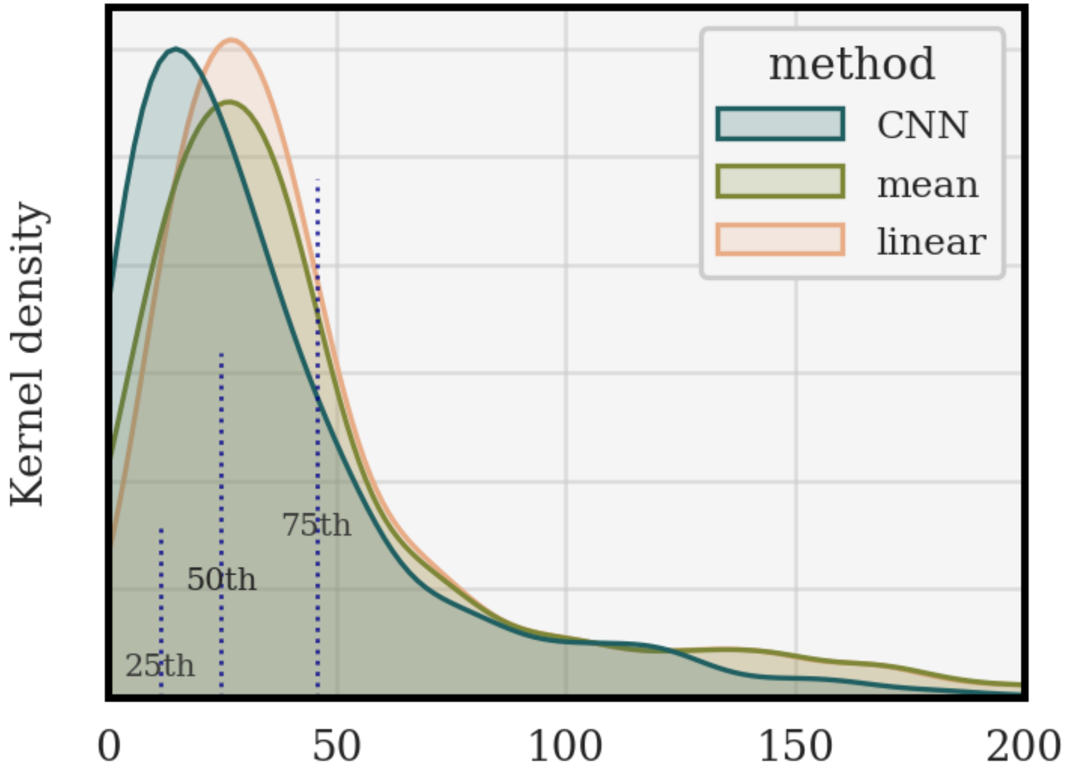
- Now investigating the use of NO2 images to support the XCO2 plume segmentation (1st results promising)



Plume inversion based on Convolutional Neural Networks

- Estimates of the total emissions from the source
- Until recently, encouraging results when training the CNN with sets of images including the targeted source

Inversion results corresponding to relative errors on hourly emission from Berlin when using a CNN trained with XCO2 images on Berlin.



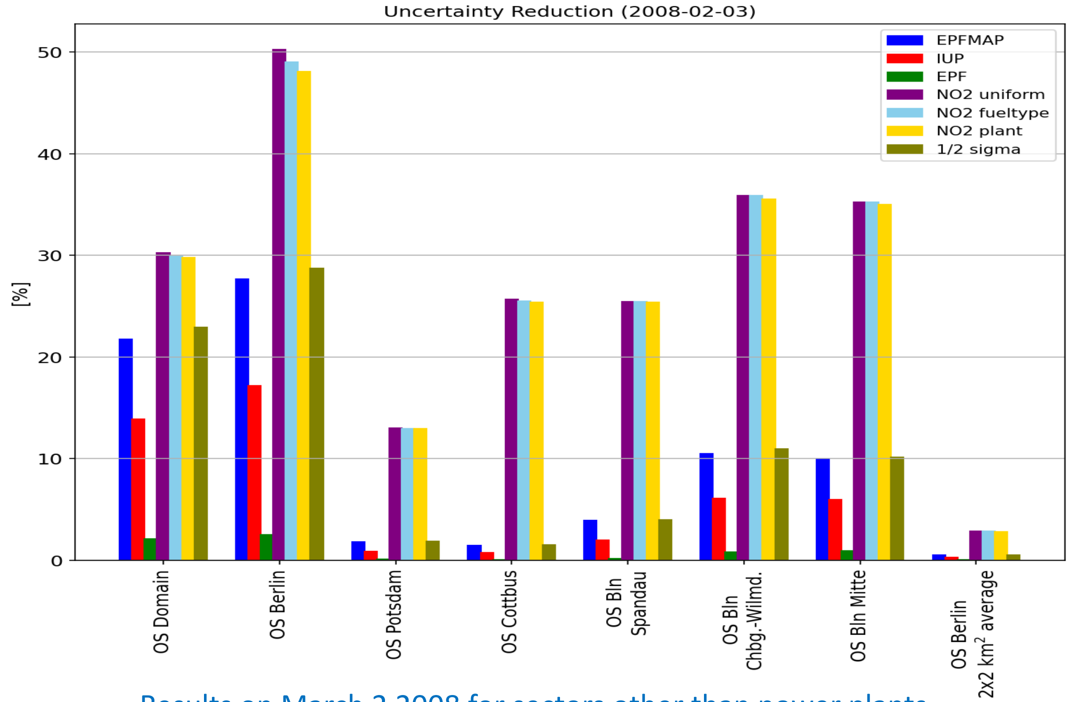
- Recent progresses and perspectives adding, in input:
  → the CNN-based segmentation results
  → the NO2 images

Subtask 4.3.2: Spatial resolution of the city emissions

Sensitivity to control vector & ability to solve for the spatial distribution of emissions within cities

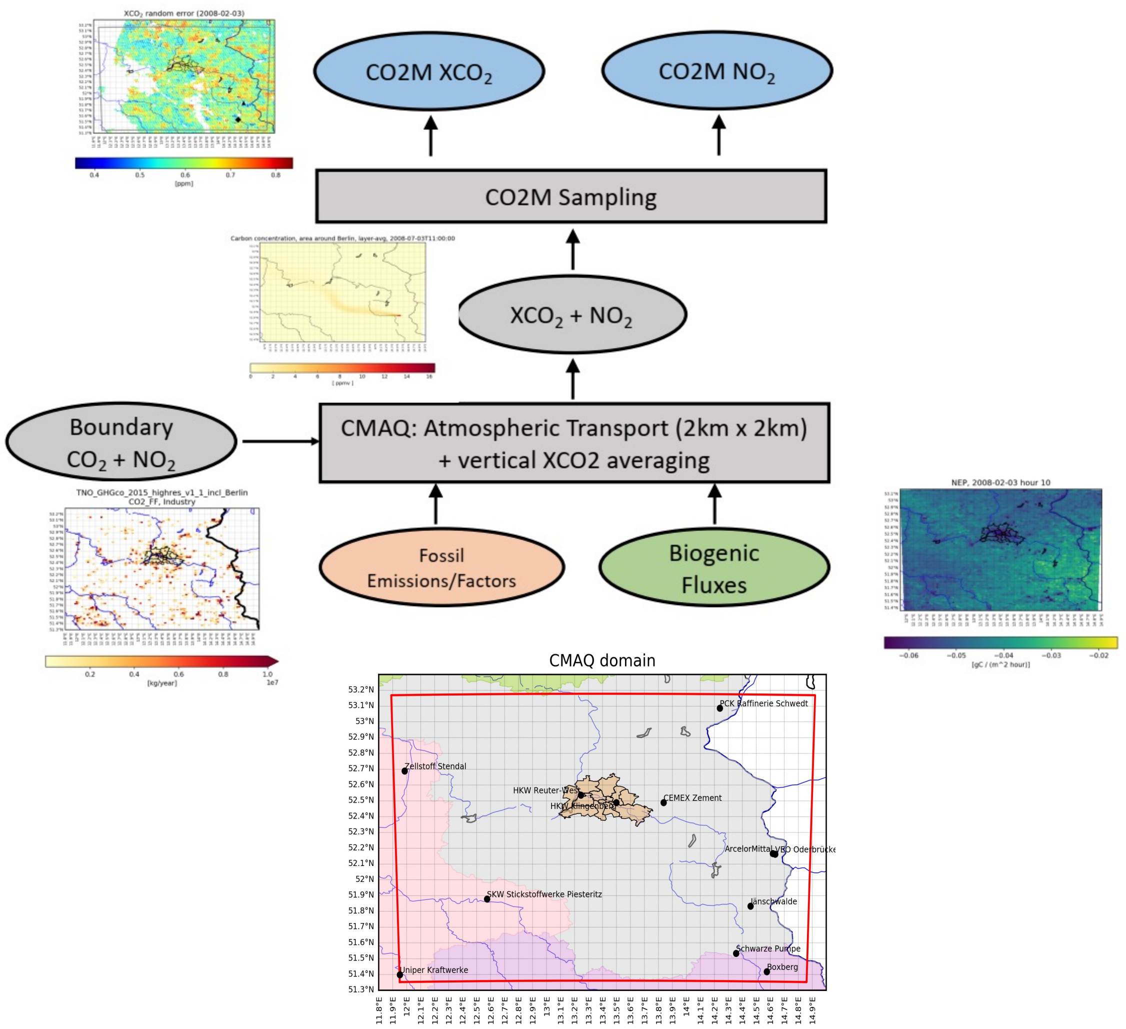
Analysis with the CCFFDAS over Berlin

Kaminski et al., 2022, Front. Remote Sens.



Results on March 2 2008 for sectors other than power plants

CCFFDAS over Berlin

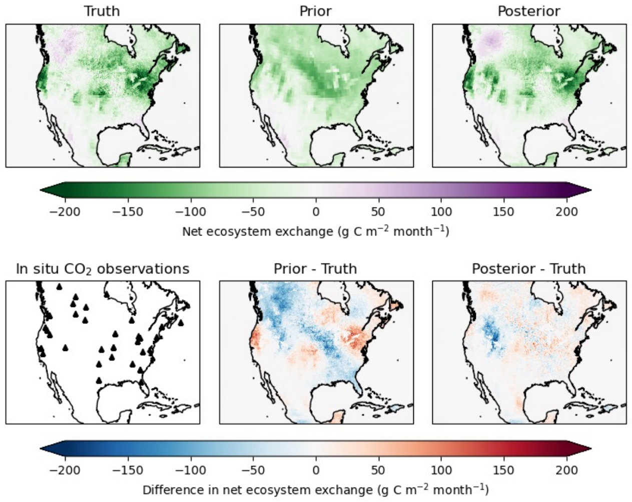


→ Ability to solve for the emission of individual districts in Berlin when using both XCO2 and NO2 images

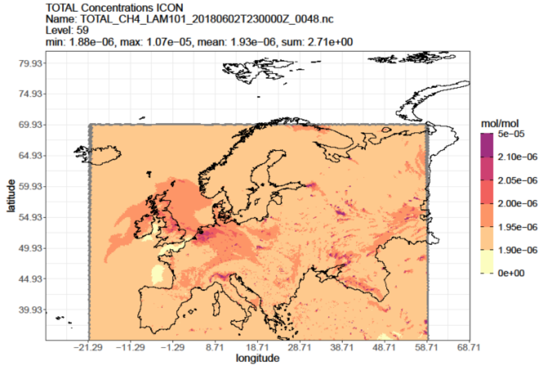
Task 4.4: National scale inversions

- Mainly for EU countries, especially for Germany, France, the Netherlands and the UK
- → CO_2 but also CH_4 inversions
- → using pseudo (incl. CO2M)/real in situ/satellite CO_2/co-emitted species data for CoCO2 ref years (2018, 2021)
- **Objective of the intercomparisons:**
- → Evaluating standard (fed by WP2-7) and country specific configs, obs networks (impact of CO2M) and methods
- → Assessing their complementarities
- Feeding WP6 & WP8: estimates for GST1 and for assimilation into prototype & supporting developments of national systems
- → **Protocol**
- → All WP2-WP7 required input available except CO2M pseudo data (coming soon)

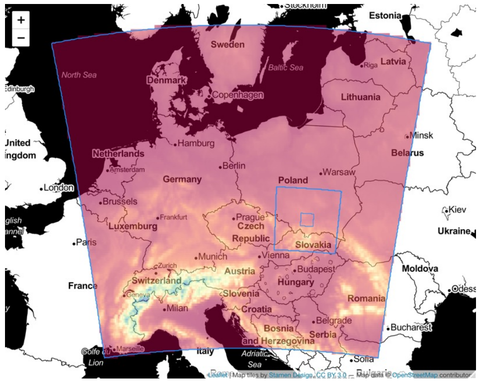
CO2 inversions with pseudo-data at ULUND



CH4 simulations at DWD



5 km – 1 km – 200 m nested configuration at AGH



Initial commitments

	France	Germany	The Netherlands	Poland	Finland	UK	USA
DLR		X	X				
UEDIN	X	X	X	X	X	X	
TNO	X	X	X			X	
DWD		X					
EMPA		X	X				
LSCE	X						
VUA			X				
FMI					X		
ULUND	X	X			X		X
ECMWF	X	X	X	X	X	X	X
AGH				X			

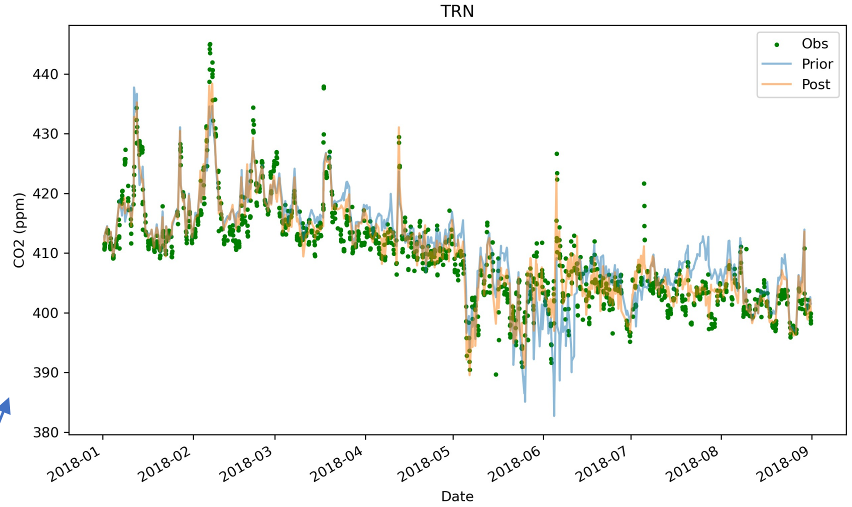
Task 4.4: National scale inversions

Inversions of anthropogenic and natural CO2 fluxes in France using in situ CO2 data

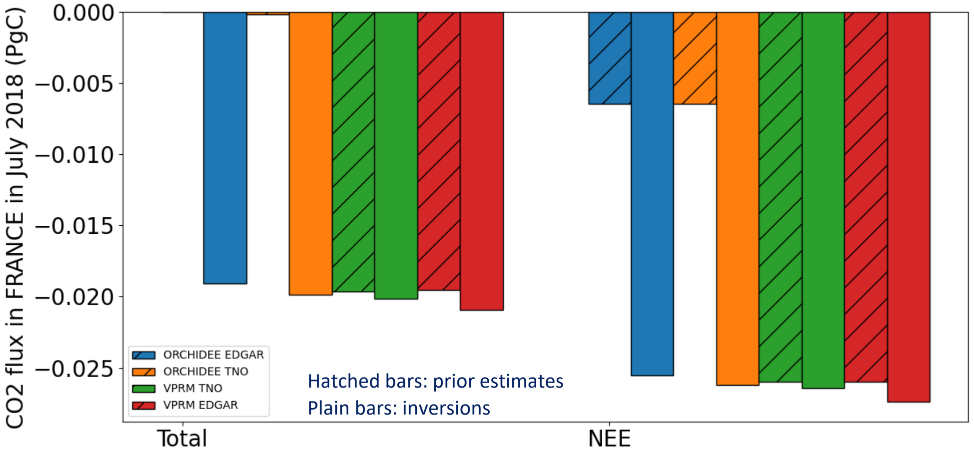
E. Potier / LSCE

- Inversions with variational mode of Community Inversion Framework (CIF) + 10 km res CHIMERE with adjoint
- Control of the NEE at 10 km / 6-h res and of the anthropogenic at the scale of admin regions and 1 day
- Tests of sensitivity to prior estimates of the NEE fluxes and anthropogenic emissions

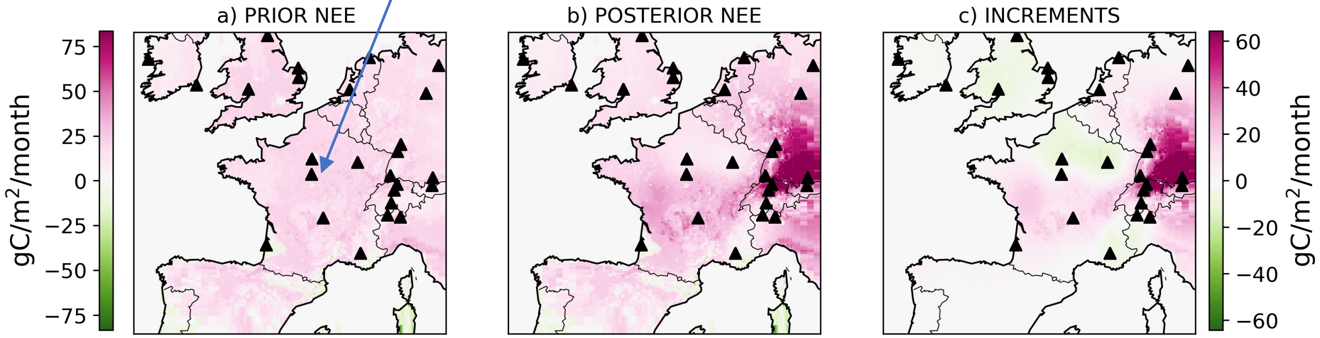
→ consistency of the maps and budgets of inverted NEE



Observed vs modelled CO2 at Trainou



NEE budget for France in July 2018

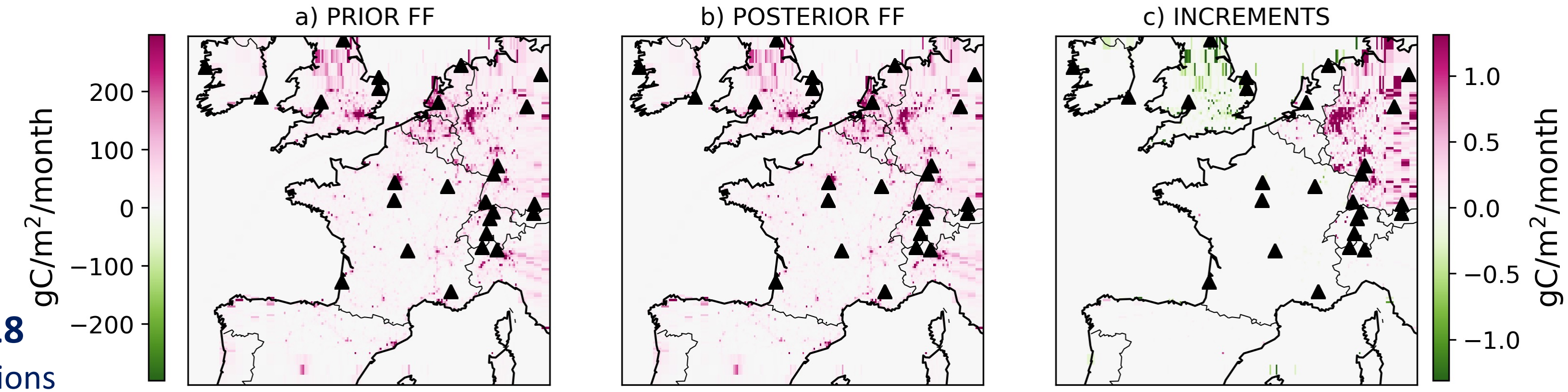


10 km resolution maps of NEE in Feb 2018
when using VPRM as prior estimate of the NEE

Inversions of anthropogenic and natural CO2 fluxes in France using in situ CO2 data

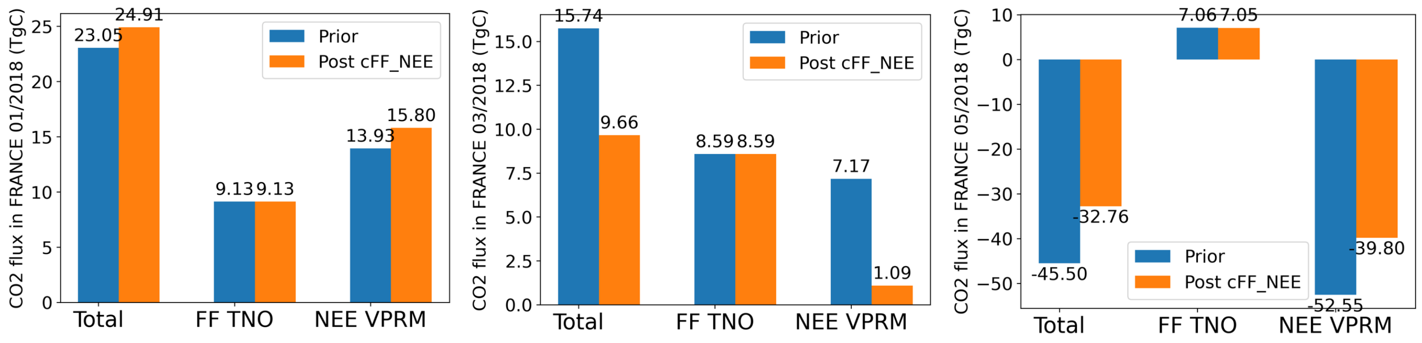
E. Potier / LSCE

- Lack of sensitivity and thus correction to anthropogenic emission estimates

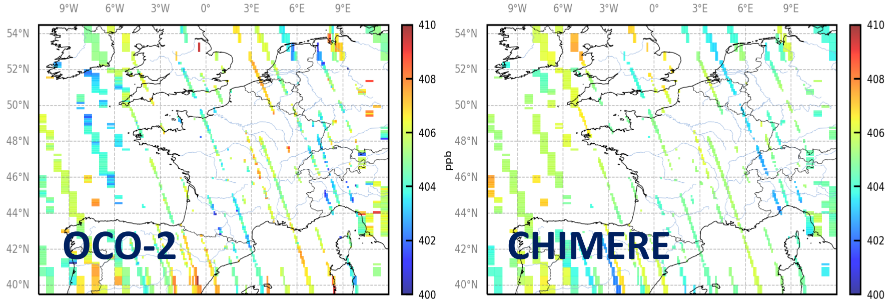


10 km resolution maps of the anthropogenic CO2 emissions in Feb 2018
when using TNO as prior estimate of the emissions

Results for Jan, March and May



- Next tests include the assimilation of OCO-2 XCO2 data



Observed and simulated OCO-2 XCO2 data in July 2018

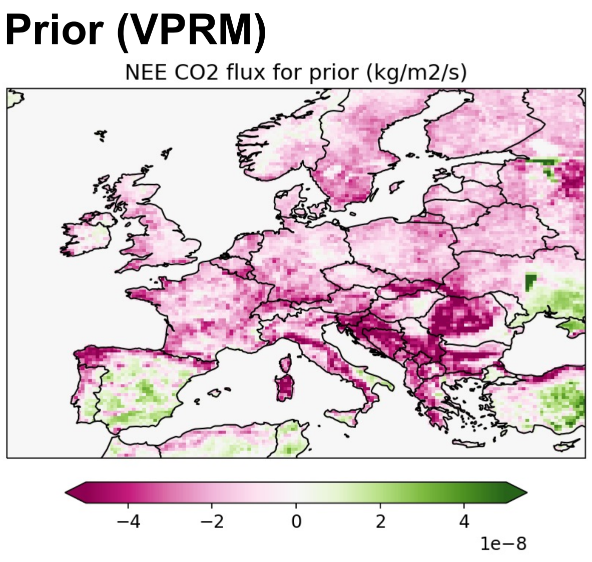
Task 4.4: National scale inversions

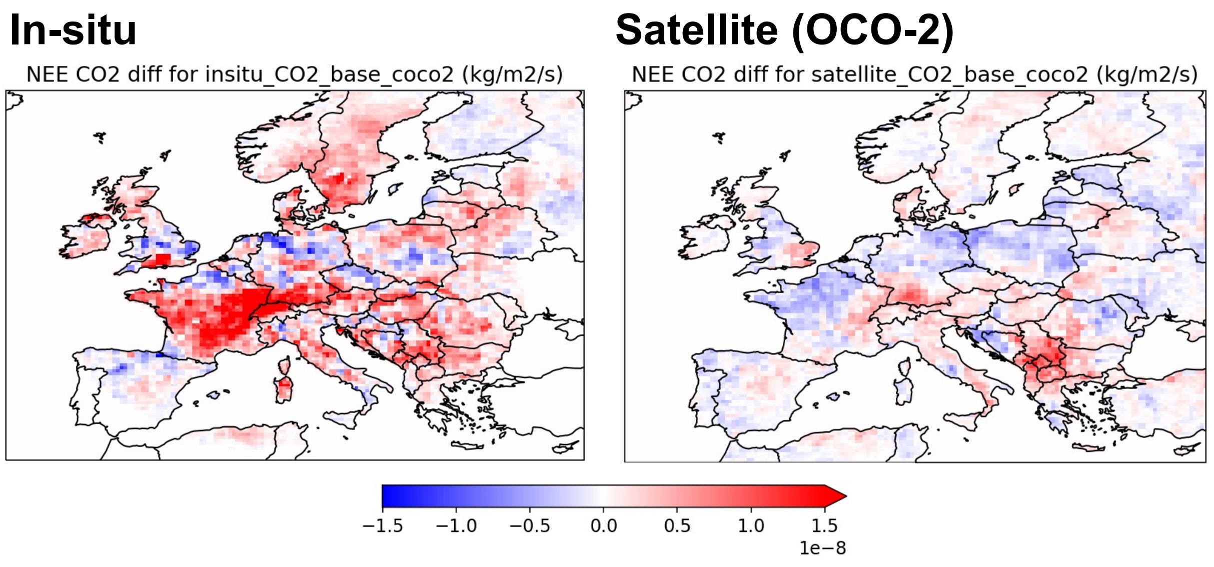
Inversions of anthropogenic and natural CO2 fluxes in Europe using CO2 / XCO2 data

T. Scarpelli / UEdin

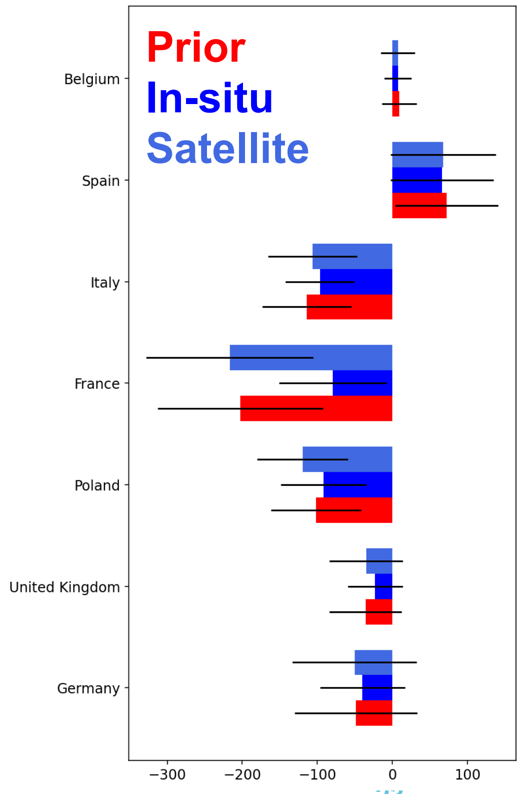
- Inversions based on EnKF (100 members) and GEOS-Chem model (0.25°x0.3°)
- Separate control of natural and anthropogenic fluxes
- Current tests assimilating in situ CO2 and satellite (OCO-2) XCO2 separately

CO2 NEE for 2018





National CO2 fluxes for 2018 (Tg)

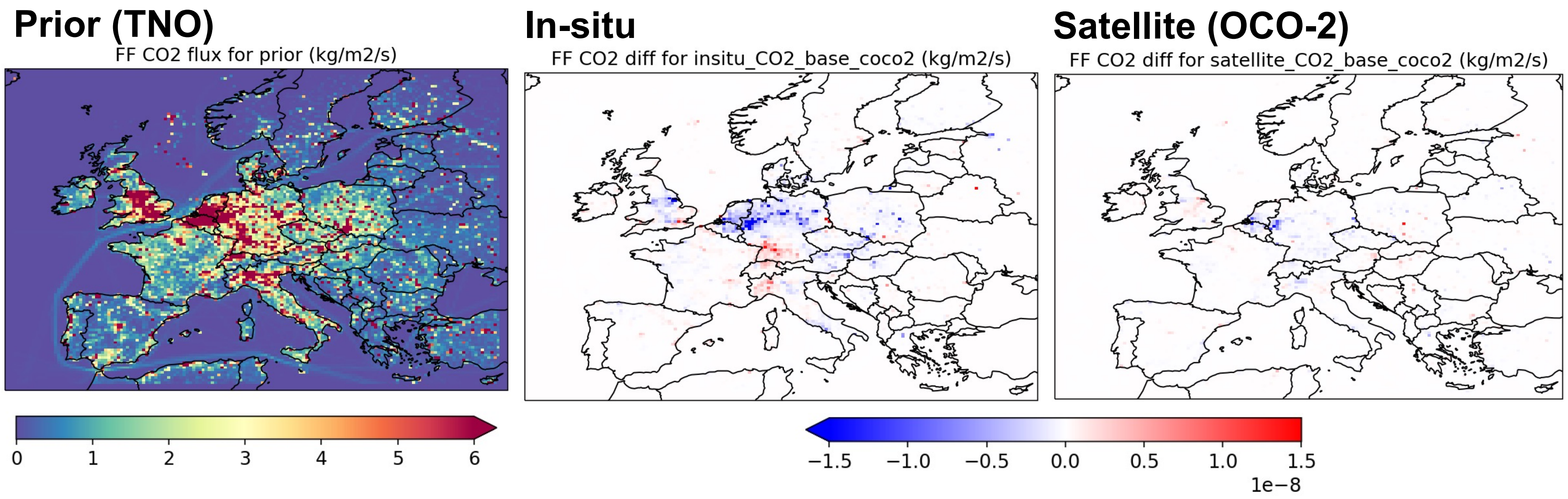


Inversions of anthropogenic and natural CO_2 fluxes in Europe using CO_2 / XCO_2 data

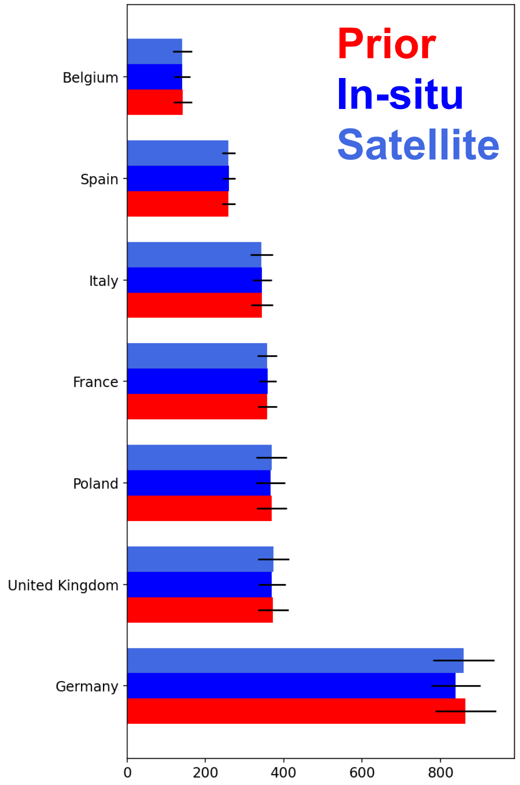
T. Scarpelli / UEdin

- Lack of correction to anthropogenic emissions
- → Need for co-emitted species
- → On-going experiments with co-assimilation of satellite CO data

CO2 anthropogenic emissions in 2018



National CO2 combustion emissions in 2018 (Tg)



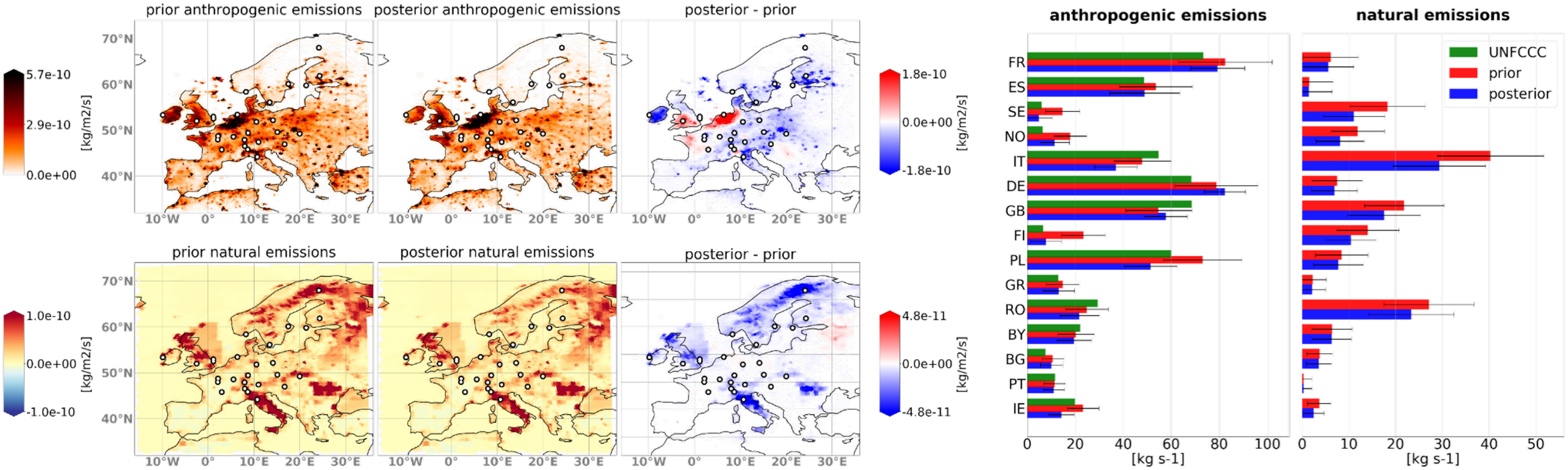
Task 4.4: National scale inversions

Estimation of European CH4 emissions

M. Steiner / EMPA

- Inversions based on ICON-ART-CTDAS (Ensemble Kalman Smoother)
- Separate control of anthropogenic and natural emissions
- On-going set-up of ICON-ART-CTDAS inversions of CO2 fluxes

2018 annual mean: maps of emissions & country scale budgets

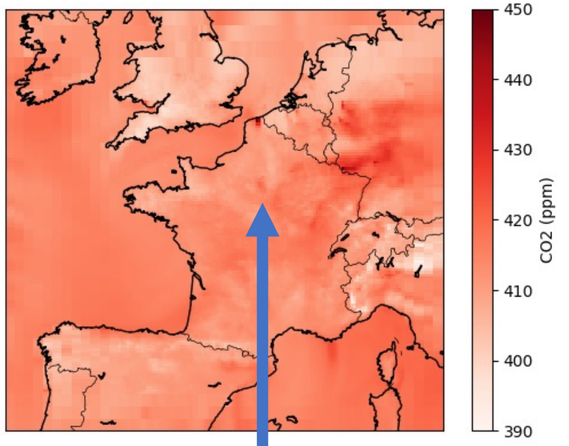


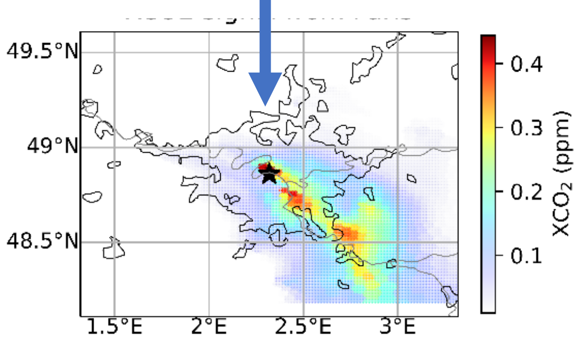
Task 4.5: Guidance & synthesis of the local and regional estimates

Synthesis of WP4, confronting results from local & national scale inversions

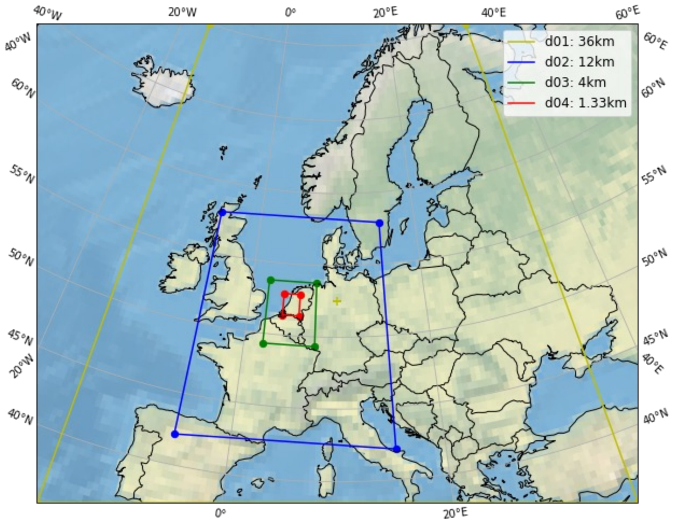
- Perspective on the use of high res model for local scale inversions from T4.1-3
- Reconciliating instant / local and national estimates: tests cases covered by local inv. (T4.2-3) and gridded national inv. (T4.4) and nested configurations
- Benchmarking test cases and criteria, guidance for the multiscale prototype in WP6 and the development of local, regional or nested systems

Surface CO_2 over France at 10 km res (E. Potier, LSCE)

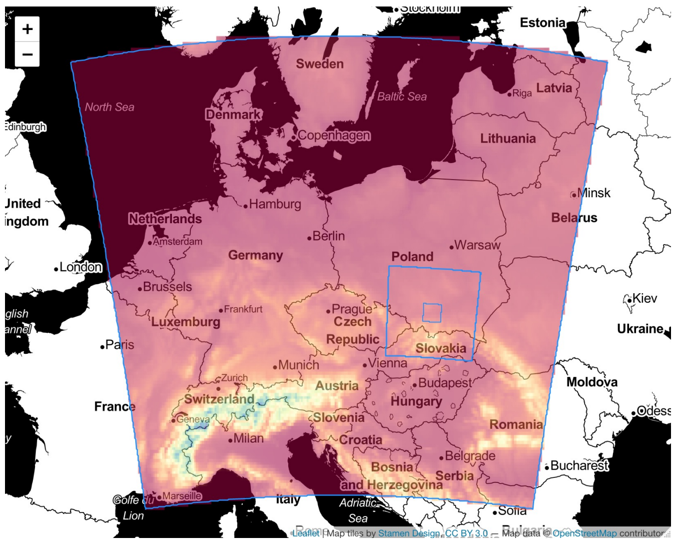




XCO_2 over the Paris area at 1 km res (Sim by J. Lian; Fig. by A. Danjou, LSCE)



Nested configuration at VUA



5 km – 1 km – 200 m nested configuration at AGH

WP4 Deliverables

D4.1 Definition of simulation cases and model systems for building a library of plumes (lead: WU)	M06	Done
D4.2 Assessment of plume model performance (lead: Empa)	M24	On time
D4.3 Documentation of plume detection and quantification methods (lead: Empa)	M12	Done
D4.4 Benchmarking of plume detection and quantification methods (lead: FMI)	M24	Delay 1-2 Mt
D4.5 Perspectives on the use of atmospheric transport models for local scale inversions (lead: ENPC)	M26	In prep.
D4.6 Intercomparisons of national-scale inversions (lead: MPG)	M34	
D4.7 Ensemble of estimates for assimilation into prototype (lead: UEDIN)	M30	
D4.8 Synthesis and recommendations (lead: CEA)	M36	

Perspectives for the final year

- Finalization of the main activities at local scale: tasks 4.1 and 4.2 and D4.5 (based on results from task 4.3)
- **T4.4 national scale inversions: Including co-emitted species in inversions of CO2 fluxes, experiments with pseudo CO2M data, sensitivity tests and inter-comparisons**
- Sending results from T4.4 national scale inversions for assimilation into multi-scale prototype in WP6 (D4.7)
- Analysis with T4.3 / T4.4 nested national to city scale configurations to feed the synthesis in T4.5 (D4.8)
- **Synthesis**
- Regular and fruitful meetings at WP and task levels sine the beginning of the project: will be maintained