Co-ordinated by ECMWF

CoCO2
Prototype system for a Copernicus CO_2 service

WORK PACKAGE 5: CONNECTING SCALES AND UNCERTAINTIES

1st General Assembly

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(ECMWF, EMPA, ICOS ERIC, CEA, MPG, TNO, ULUND, VUA, WUA, CMCC, FMI, iLAB, MF)

16/11/2021

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WP5 Rationale

WP Objective:

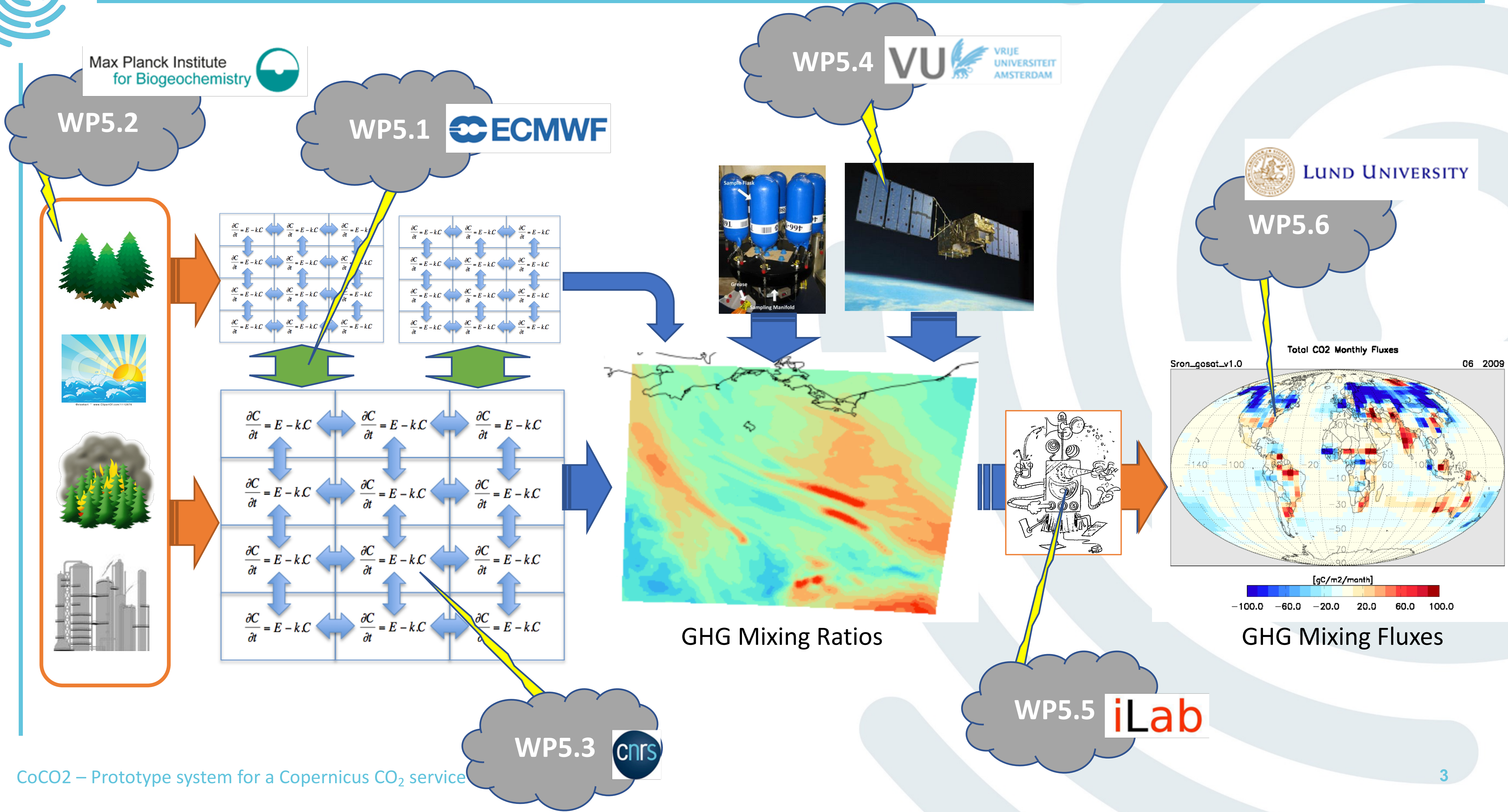
Improve the representation of uncertainties in inversions, in order to:

- Obtain realistic a posteriori flux / parameter uncertainties
- Optimize the weighing of information elements that are used to constrain the inverse problem
- Facilitate the information exchange between sub-systems operating at different scales (e.g. global system and high-resolution local systems)

Focus & approach:

- Focus on the following aspects: boundary conditions, sampling biases, transport uncertainty, inversion design options, posterior uncertainty estimation
- Methods: Real data / OSSE, Global / Regional models, Benchmarking using independent Obs.

WP5 structure



Task deliverables & milestones

Deliverable	Title	Lead	Due
D5.1	Proof-of-concept for multi-scale global IFS prototype	ECMWF	**M36**
D5.2	Toolbox to derive customized model forcing data and for assessing errors of simulated terrestrial CO2 fluxes from data base of biogenic CO2 flux measurements	MPG	**M24**
D5.3	Quantification of transport errors and database of optimized fluxes and simulations for an ensemble of models and inversion set-up	CEA	**M30**
D5.4	The representation of CO2M satellite retrieval uncertainty in inverse modelling	VUA	**M33**
D5.5	Impact of System Design on Emission Estimates	iLab	**M33**
D5.6	Quantification of uncertainty ranges from European multi-model inversions and ways to benchmark inversion systems	ULUND	**M33**
D5.7	Summary report of the WP5 activities for year one	ULUND	**M12**
MS11 (5.1)	CIF working and tested with six of eight transport models	CEA	**M12**
MS12 (5.2)	Database of optimised regional fluxes based on ensemble of IFS-driven boundary conditions = T5.3	CEA	**M24**
MS13 (5.3)	Best-practice on benchmarking atmospheric transport inversions	ULUND	**M24**

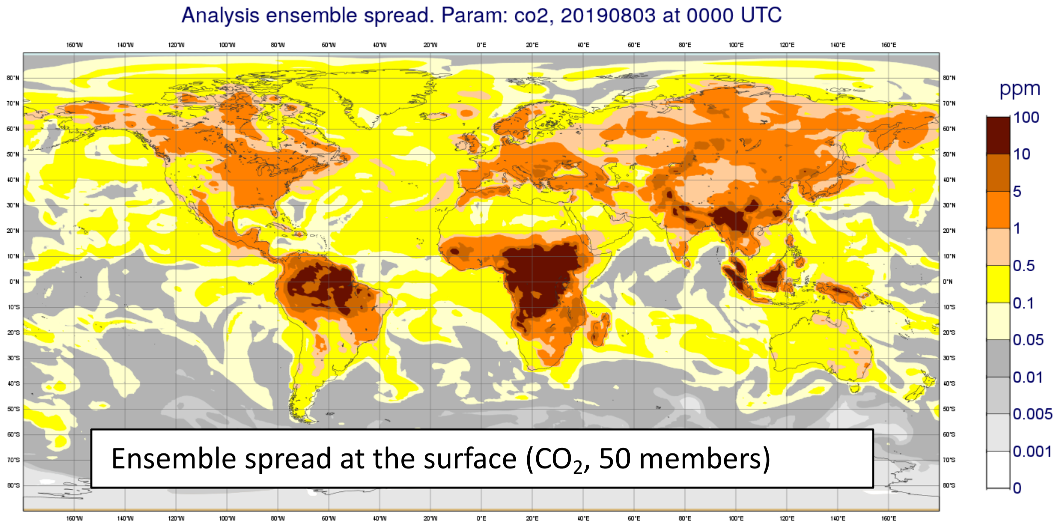
T5.1: Information transfer Global - Local

Progress on Ensemble of Data Assimilation

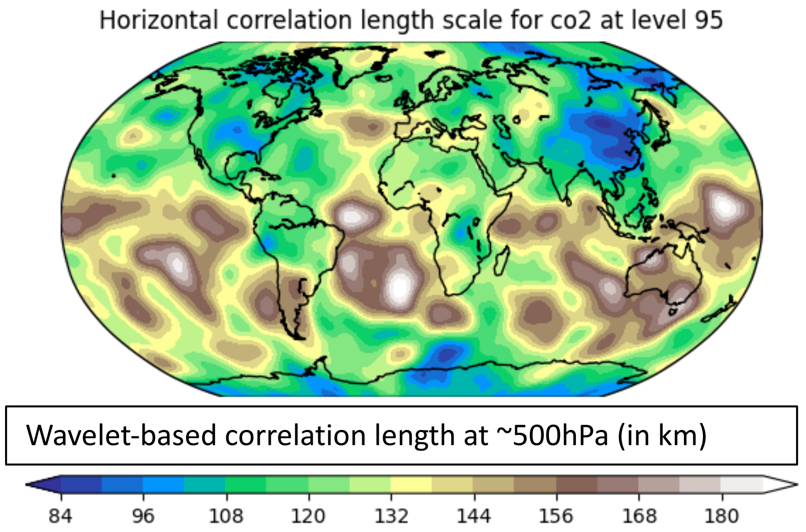
- We are testing an **Ensemble** of Data Assimilation for GHG (CO_2 and CH_4). This will result in a **better estimation of uncertainty** based on weather-dependent information.

- The new ensemble can be used as ensemble of **boundary conditions** for other local inversion models (cf. task 5.3, CIF) to improve uncertainty estimates in nested configurations.

- The wavelet method (already used for the NWP) will allow us to model spatially-varying emission error **covariances** globally, a key capability for high-dimensional top-down inversions.



Ensemble spread at the surface (CO_2, 50 members)



Wavelet-based correlation length at ~500hPa (in km)

N.B. Emissions/surface fluxes **not** included at this stage. The ensemble is generated by perturbing only the model physics and the observations, and independent analyses are produced to sample to posterior errors.

Task 5.2: Assessing and quantifying errors of biogenic CO_2 fluxes

Hold several discussion meetings and benchmarking workshop (notes on confluence), the main outcomes are:

- Recommendation for a multi-faceted and diversified evaluation approach across scales
- Adapting modelevaluation.org infrastructure from Gab Abramowitz for benchmarking at flux tower sites (ongoing by Jung/Nelson, Abramowitz, Papale, Vermeulen/Karstens)
- Tailored OSSE experiments to identify key metrics for effective CO2MVS benchmarking (started by Kaminski, Scholze, Jung)

Work on required flux tower data and pipelines for benchmarking:

- Acquisition and processing of remotely sensed model inputs
- Improved gap-filling of precipitation
- Improved and complementary flux tower data quality control

Two related manuscripts are in preparation

T5.3 Transport model uncertainties & CIF

MS11 (due M12): "*CIF working and tested with six of the eight following transport models (CHIMERE, LMDZ, TM5, FLEXPART, WRF-CHEM, LOTOS-EUROS, STILT, COSMO-GHG)*":

- most models mentioned in the proposal are now implemented: CHIMERE, LMDZ, TM5, FLEXPART (NILU's and EMPA's versions), WRF-Chem
- additional models to come: STILT and LOTOS-EUROS
- COSMO-GHG postponed to longer term

CIF is used in VERIFY CH_4 inter-comparisons with CHIMERE and FLEXPART (NILU and EMPA)

Task 5.4: Accounting for correlated uncertainty in satellite data

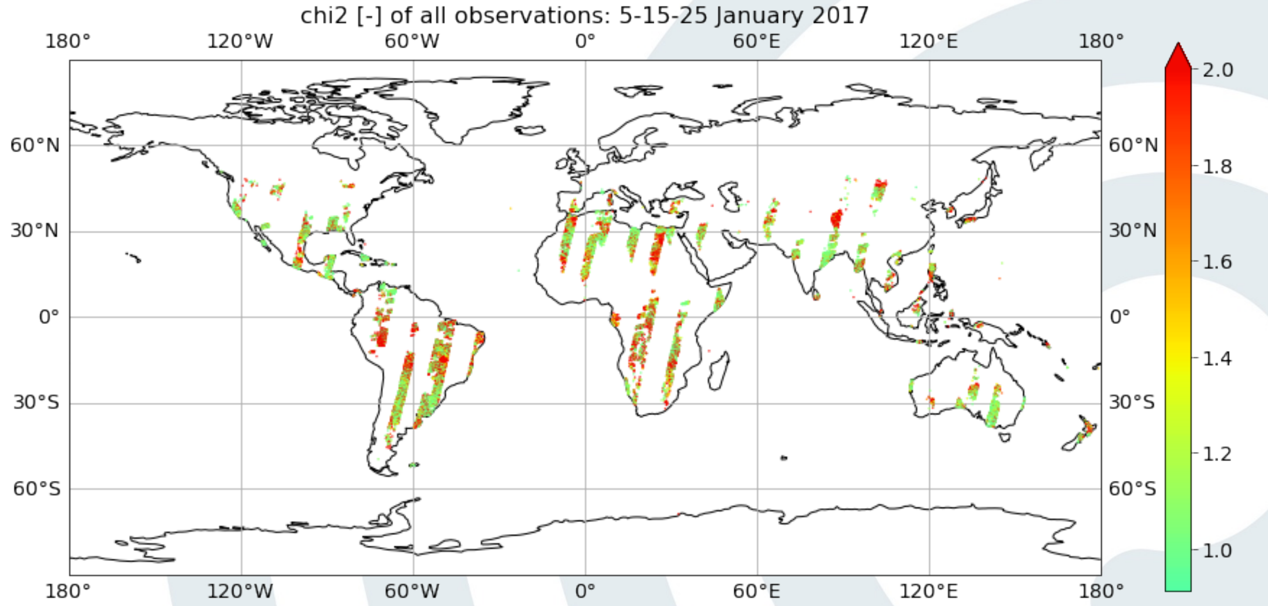
CO2M pseudodata (source: SRON)

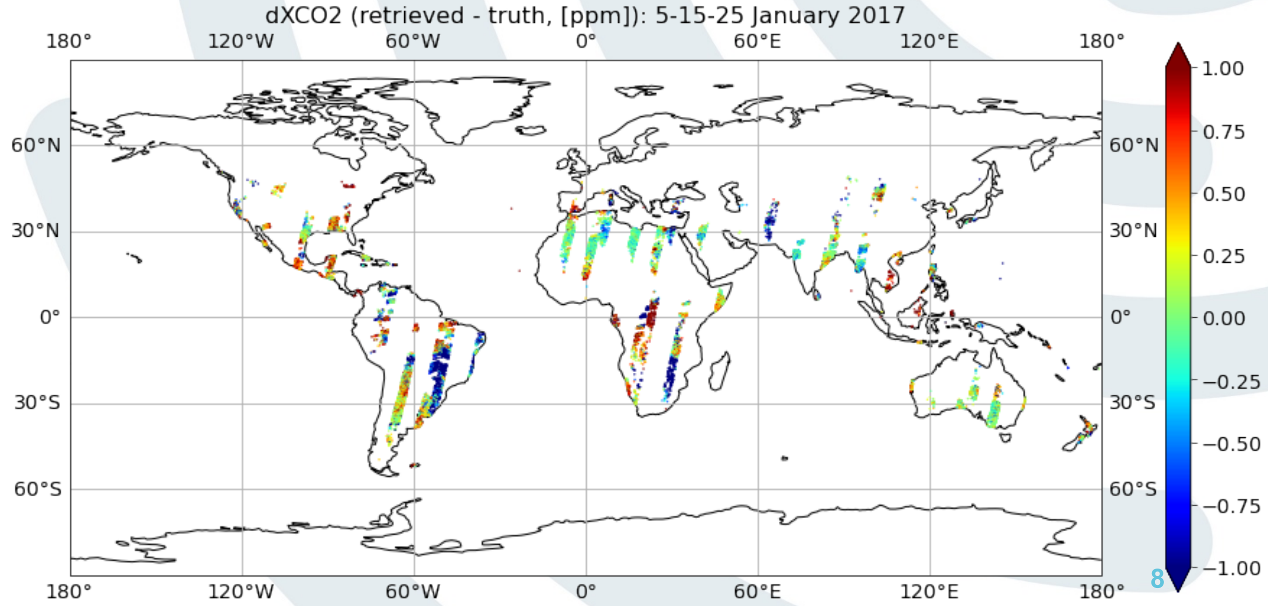
- RemoTAP retrieval algorithm applied to simulated atmosphere,
- for 60 days in 2017, 1% of the pixels

Winter:

→ Goodness-of-fit filtering (chi2 < 2): 30.4% of observations discarded

→ RMSE = 1.115 ppm, bias = -0.13 ppm





Task 5.4: Accounting for correlated uncertainty in satellite data

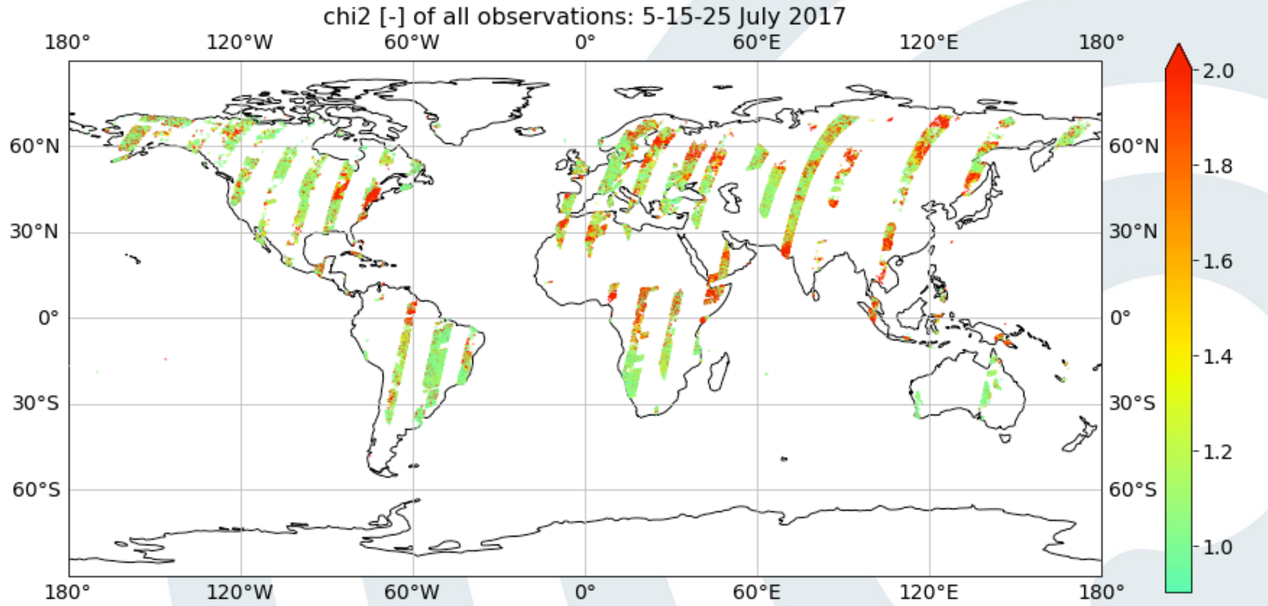
CO2M pseudodata (source: SRON)

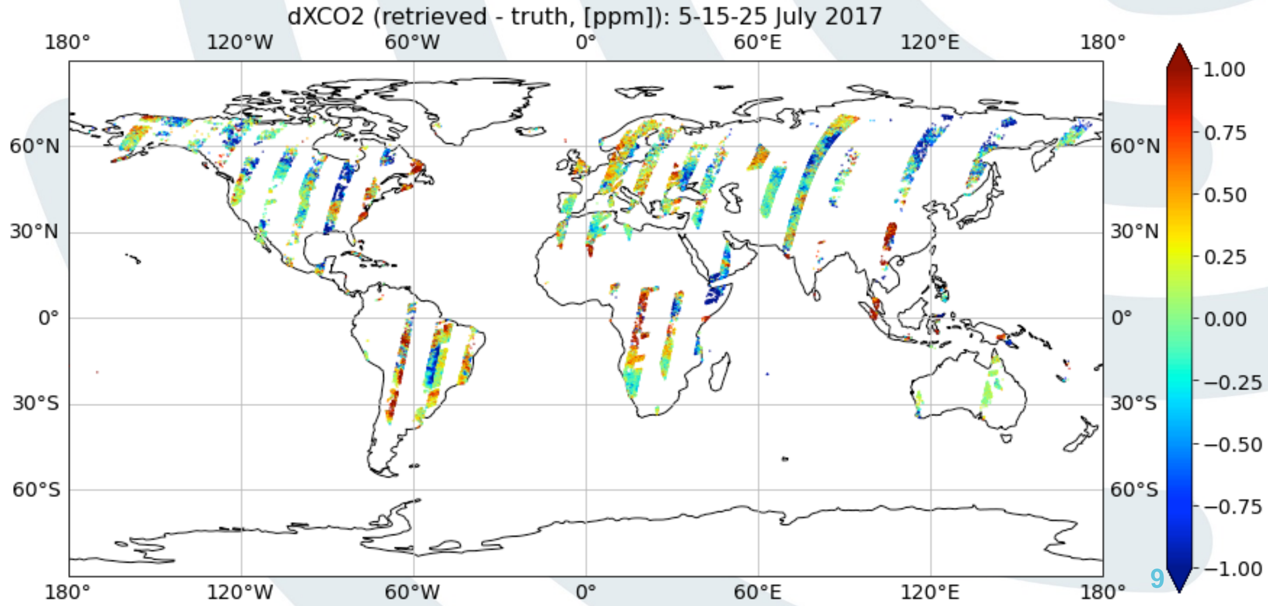
- RemoTAP retrieval algorithm applied to simulated atmosphere,
- for 60 days in 2017, 1% of the pixels

Summer:

→ Goodness-of-fit filtering (chi2 < 2): 21.5% of observations discarded

→ RMSE = 0.725 ppm, bias = 0.0025 ppm





Task 5.5: QND and data assimilation sensitivity studies

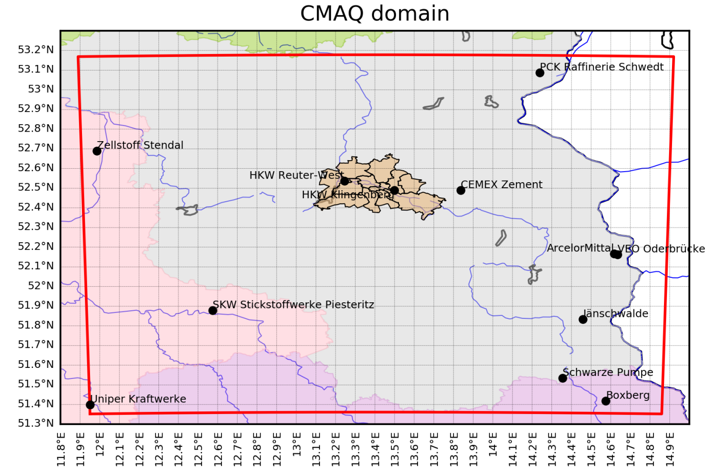
Objective: How important are NO2 observations (complementary to XCO2 observations) to estimate Emissions of a Megacity in CCFFDAS

Subsequent plots show:

Prior/Posterior uncertainty for energy generation and “other sector” (all remaining fossil fuel emissions).

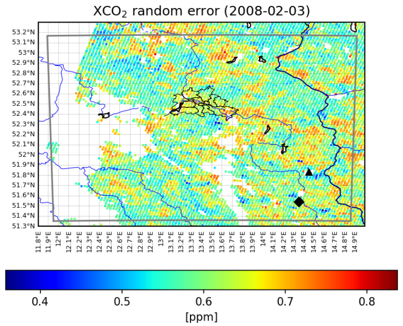
On a day in winter

- Emissions over 24 hours preceding the CO2M overpass time
- 2 km x 2 km resolution of 200 km x 200 km domain around Berlin
- 20% prior uncertainty for prior fossil fuel emission (per power plant, at city level: 52.8% per pixel for other sector), each parameter of the natural flux model, and ~1ppm for the inflow into each lateral boundary grid cell
- 4 Cases:
  - No NO2
  - NO2: Random error 0.5 10^{15} molec/cm^2 (Lorente et al., 2019), systematic error 0.3 10^{15} molec/cm^2
  - NO2: Random error 1.5 10^{15} molec/cm^2 (MRD upper limit), systematic error 0.3 10^{15} molec/cm^2
  - NO2: Random error 0.25 10^{15} molec/cm^2, systematic error 0.3 10^{15} molec/cm^2



Task 5.5: QND and data assimilation sensitivity studies

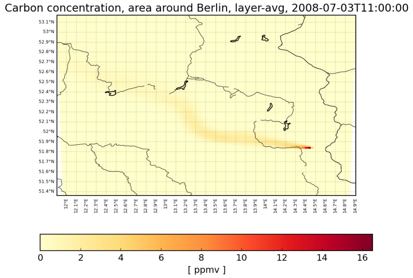
Modelling Chain



CO2M XCO_2

CO2M NO_2

CO2M Sampling



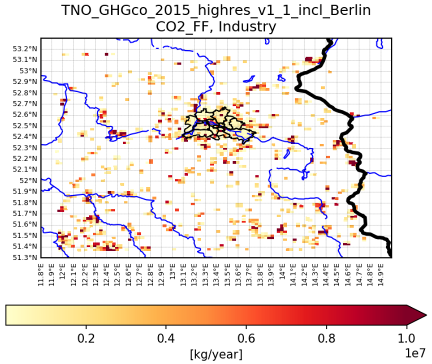
$XCO_2 + NO_2$

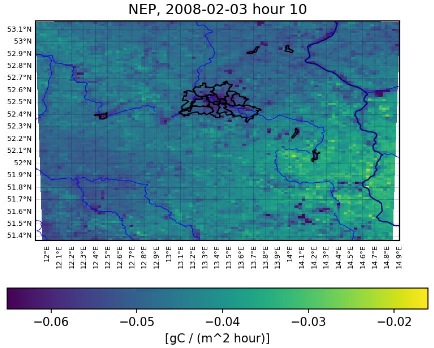
Boundary $CO_2 + NO_2$

CMAQ: Atmospheric Transport (2km x 2km) + vertical XCO2 averaging

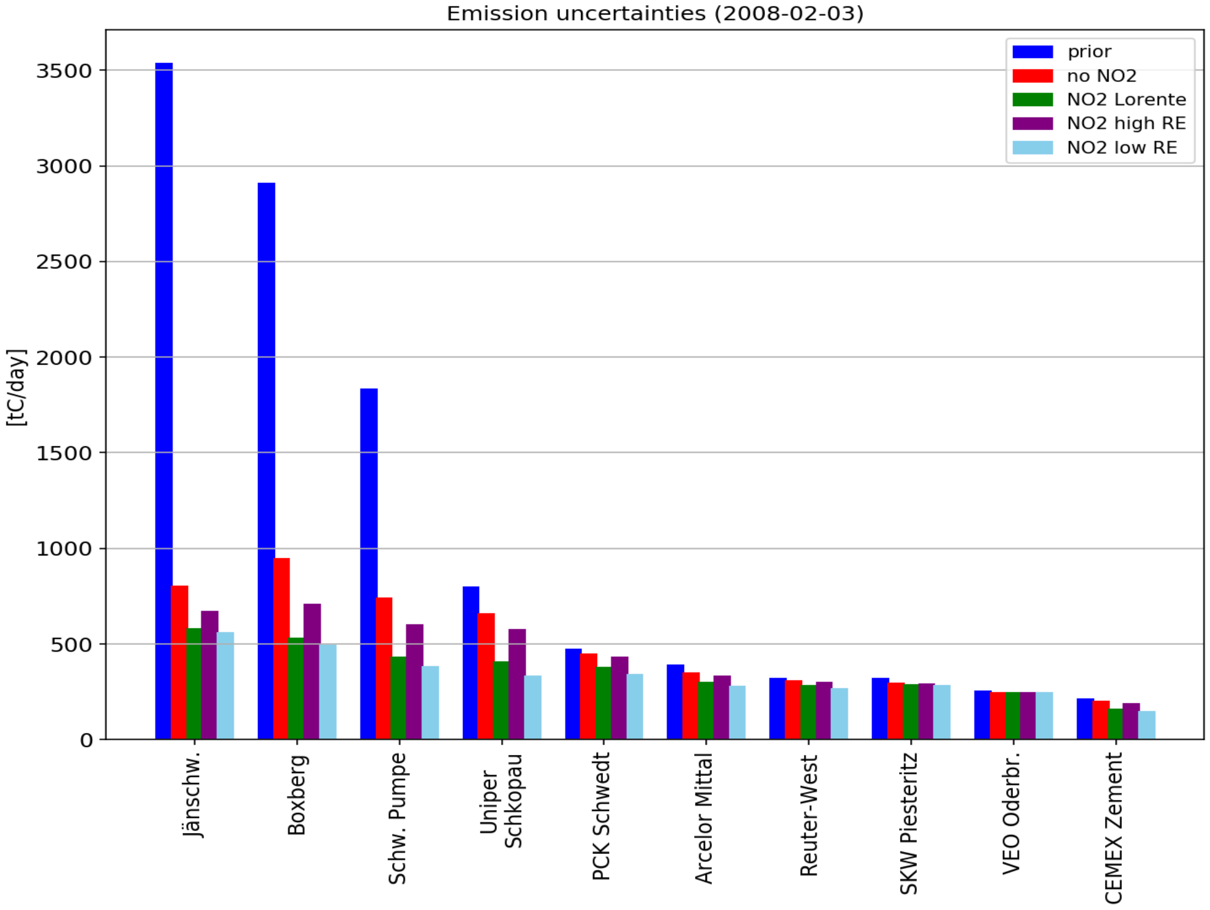
Fossil Emissions/Factors

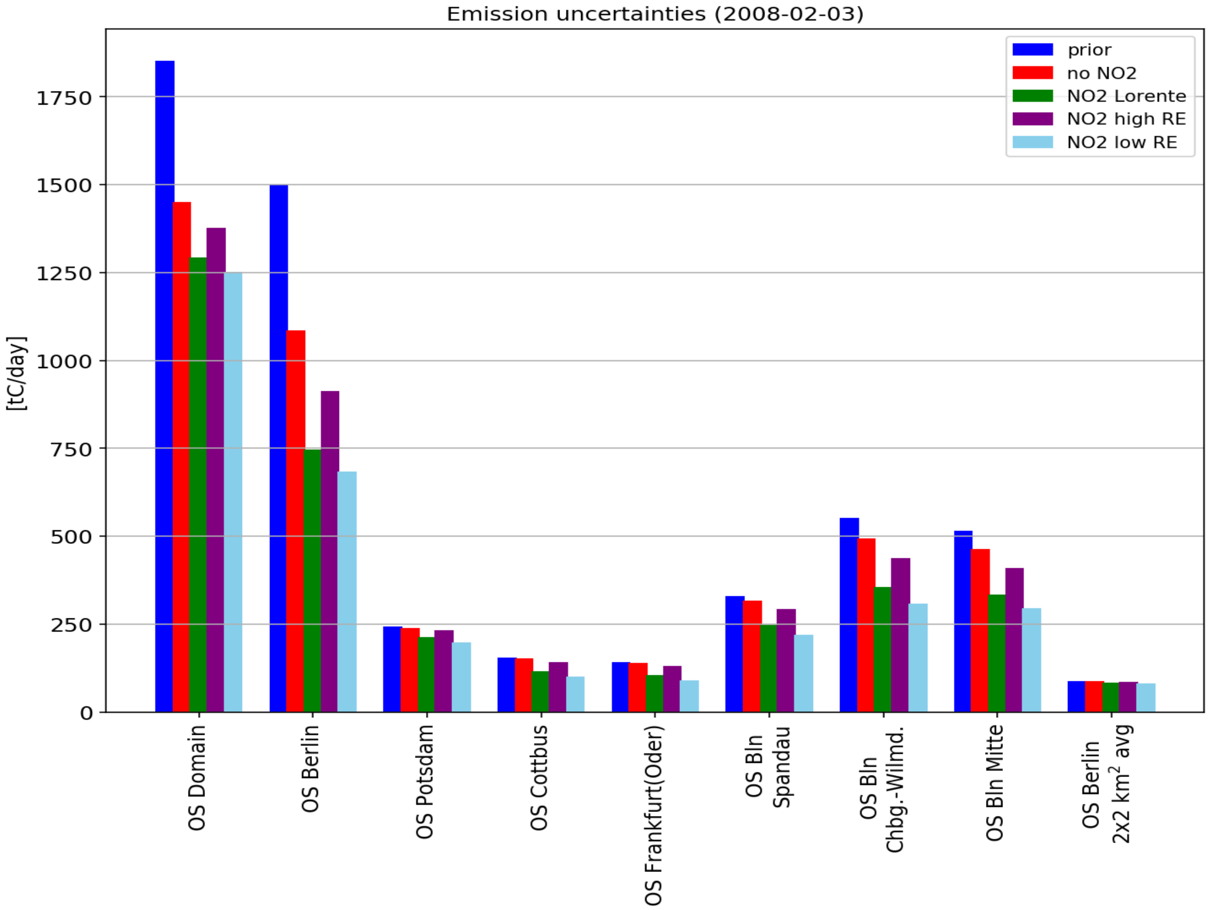
Biogenic Fluxes





Task 5.5: QND and data assimilation sensitivity studies

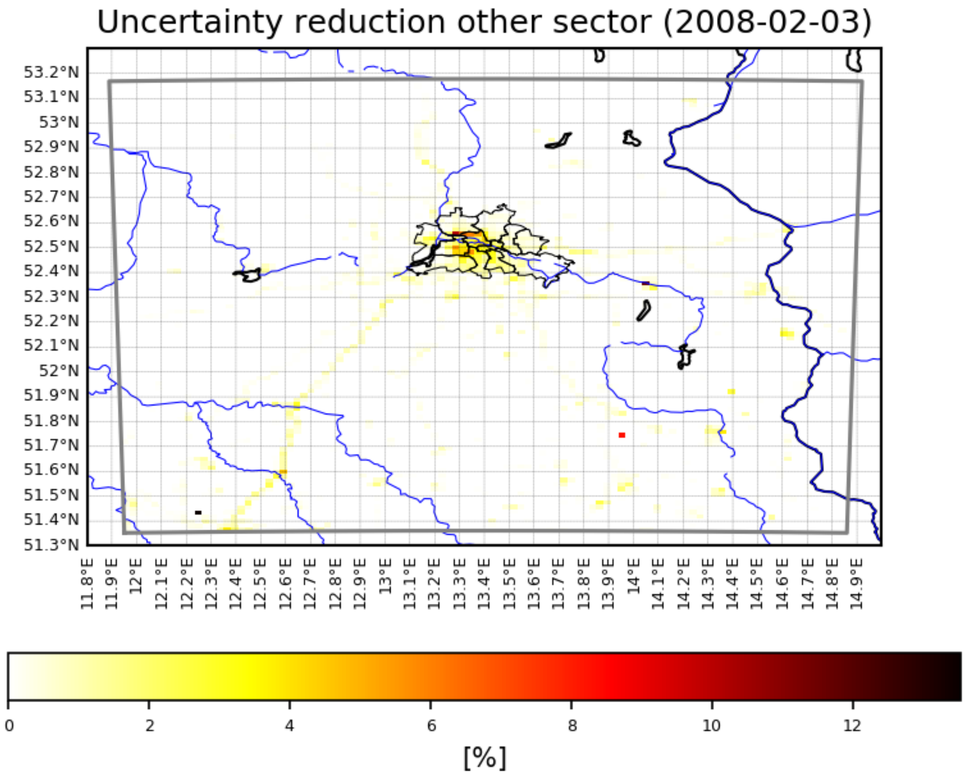


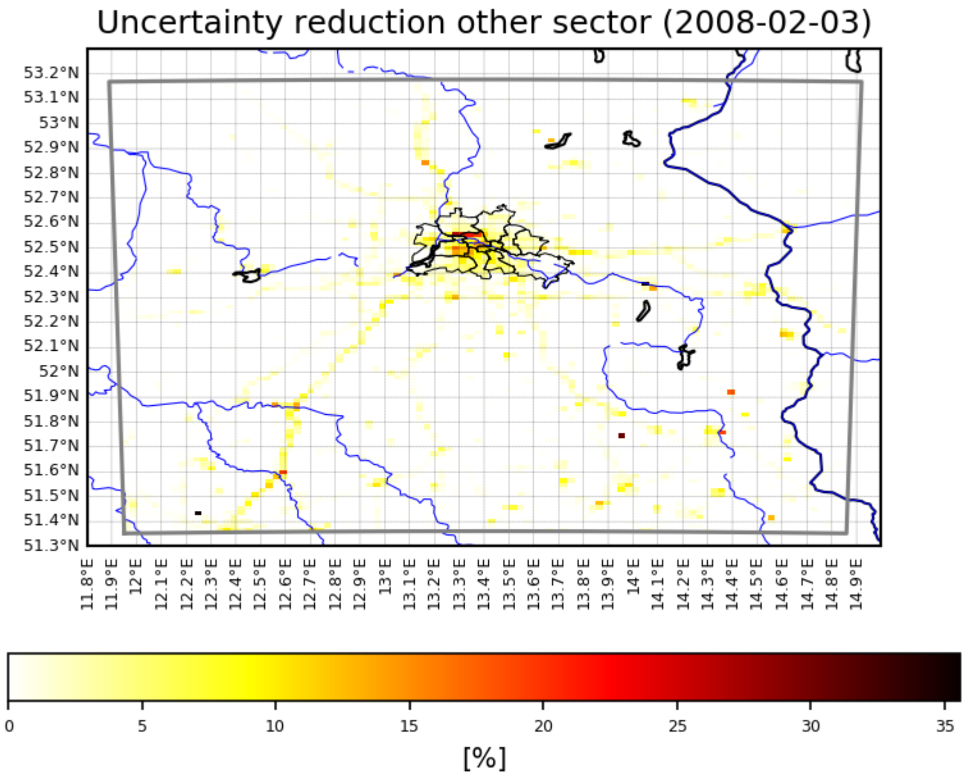


10 largest power plants in domain

All remaining emissions from domain scale (left), via city scale (second left) to pixel scale (right)

Task 5.5: QND and data assimilation sensitivity studies





Uncertainty Reduction at pixel level:
High Random Error

Uncertainty Reduction at pixel level:
Low Random Error

Task 5.5: QND and data assimilation sensitivity studies

Results:

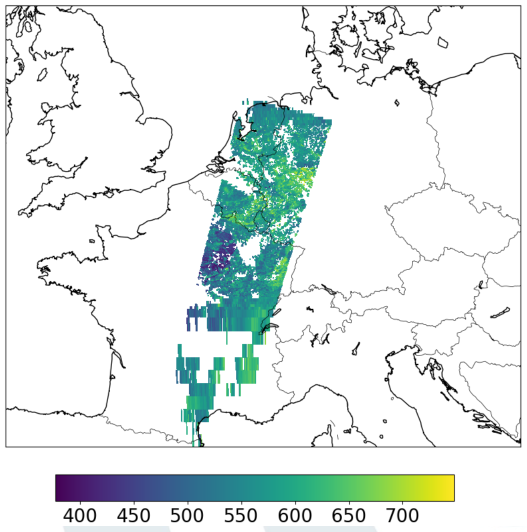
- NO_2 has strong effect on larger power plants
- With NO_2 as additional observation CO_2 prior uncertainty for entire city reduced by ~50%
- Little effect at pixel scale of 2 x 2 km
- NO_2 still useful when random error tripled
- Reduction in NO_2 random error (to level similar of systematic error) yields small benefit (extra uncertainty reduction of ~10% at city scale)
- Summer case under way (generally higher uncertainty reduction), further aspects to look at …

Fresh in the press (global CCFFDAS from CHE):
Kaminski et al., Environmental Research Letters:
Assimilation of atmospheric CO_2 observations from space can support national inventories.

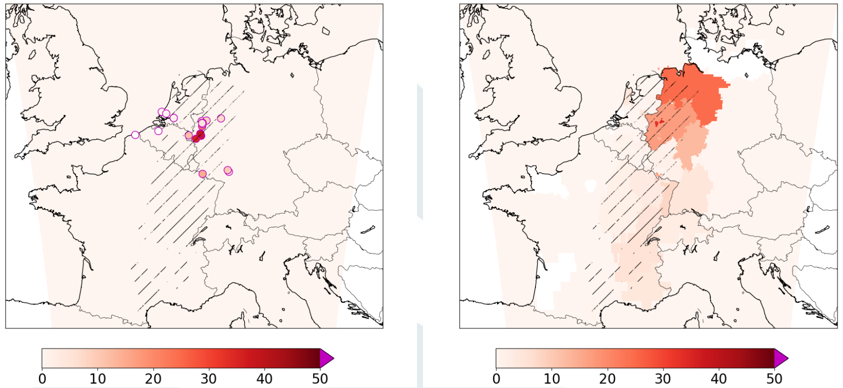
T5.5: The CO2 / ^{14}CO2 inversion system at LSCE

- System developed in CHE and ready for new sets of inversions with pseudo data:
  - Focus on Western Europe with zoom of transport model at 2 km resolution
  - Co-assimilation of CO_2 and $^{14}CO_2$ data
  - Inversion of CO_2 and $^{14}CO_2$ fluxes from FF & biofuels, nuclear power plants, and ecosystem NPP and HResp at regional to plant scale
  - Testing the complementarity between XCO2 spaceborne imagery (currently sim from IUPB / ESA-PMIF) and networks of surface CO_2 / $^{14}CO_2$
  - Analytical inversion system : based on a large ensemble of simulations of up to a few days
  - Year of study : 2015

➢ Plans to support the analysis in WP4-5 with tests including:
  - the simulation of the CO2M obs used in WP4/5
  - some surface networks used in T4.4



XCO2 spatial sampling and random noise (in ppb) for one orbit of CO2M (sim from IUPB / ESA-PMIF)



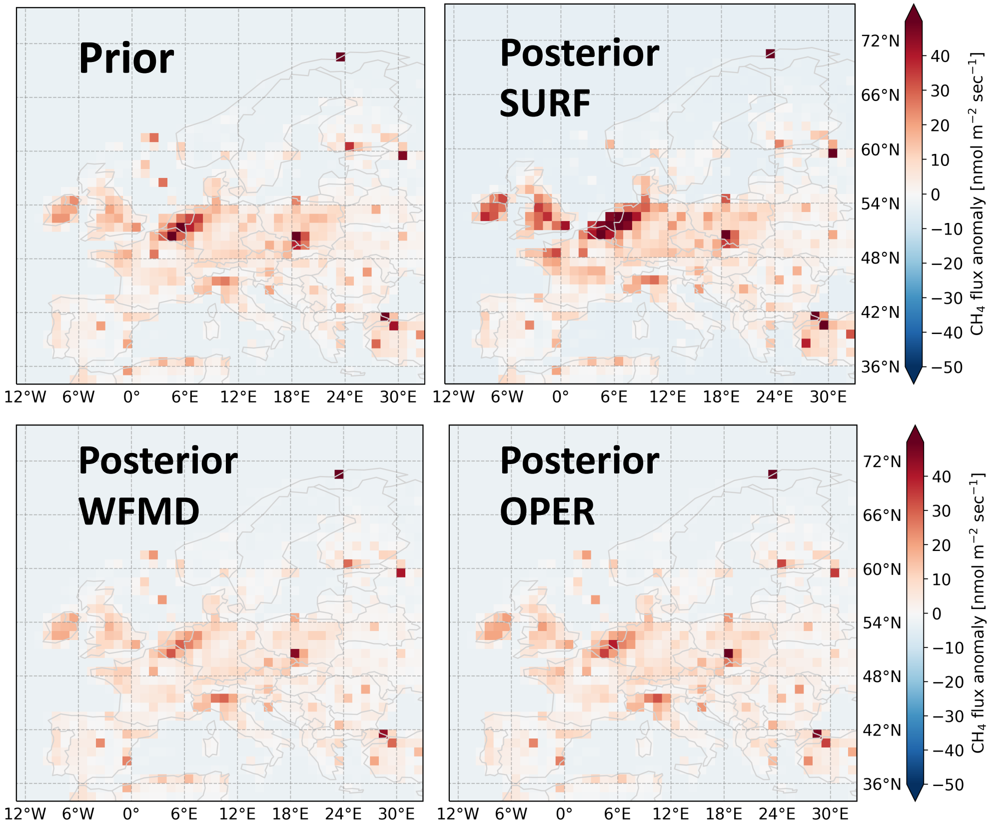
Uncertainty reduction (from ~45% prior uncertainties) in estimates of FF morning emission for large plants (left), large cities and regions (right)

T5.5: Uncertainties of posterior fluxes related to observations assimilated in atmospheric inversion (FMI)

T5.5 Evaluate uncertainties of posterior fluxes and improve their temporal consistency by assessing the impact of in-situ network, length of assimilation window, prior error description for CH_4 using the CTE-CH_4 model.

T5.6 Contribute to evaluation of atmospheric CO_2 and CH_4 concentration estimates and their uncertainties using data from surface in situ network, aircraft, AirCore, TCCON and satellites.

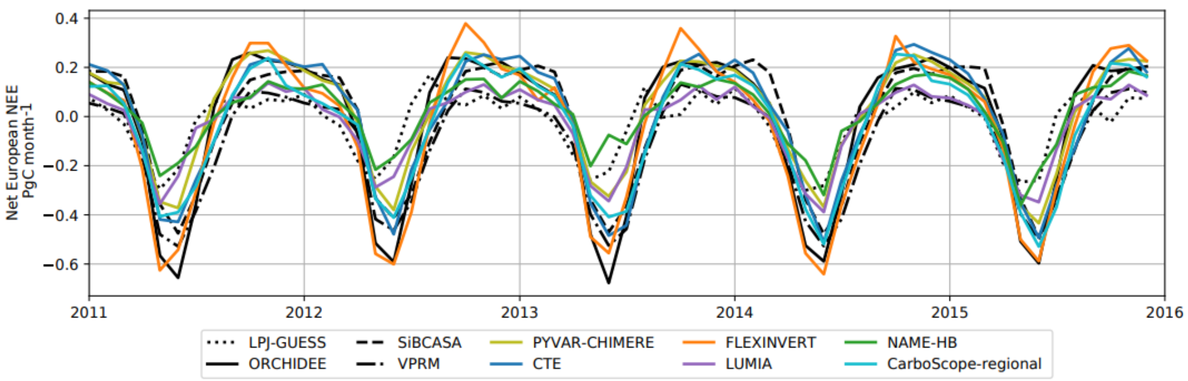
- European CH_4 fluxes are estimated using CTE-CH_4 model by assimilating data from surface in situ network and satellite (S5P TROPOMI).
- Spatial anomalies show:
  - Anthropogenic emission enhancement in central Europe
  - Emission enhancement is strong in cities
  - Emission enhancement in western Europe is largest when surface data is assimilated, and weakens when using satellite data is assimilated
  - No significant changes in location of hot spots from the prior

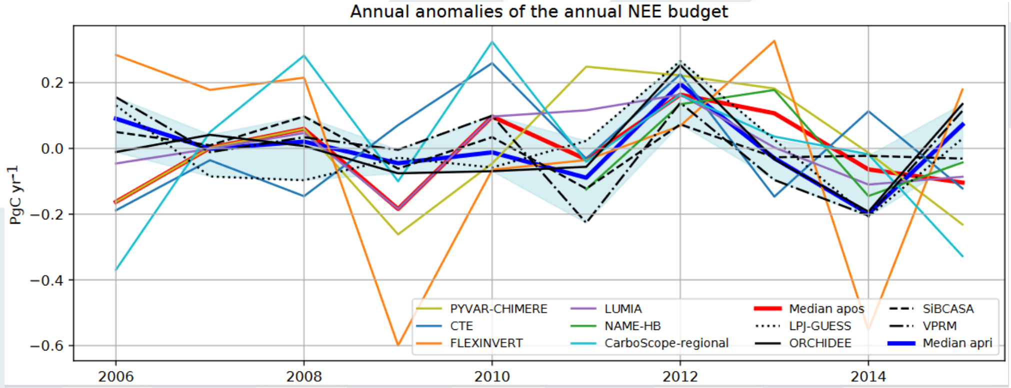


Spatial anomaly (estimates – regional mean) of prior and posterior anthropogenic fluxes over Europe, averaged over 2018
Tsuruta et al., in prep.

Task 5.6: Uncertainties in European inversions of CO_2 and CH_4

Starting point for uncertainties in CO2 inversions: EUROCOM intercomparison





EUROCOM project:

- 6 inversion systems from 6 research groups
- Different priors, transport models, inversion approaches, etc.
- Common(ish) observation database

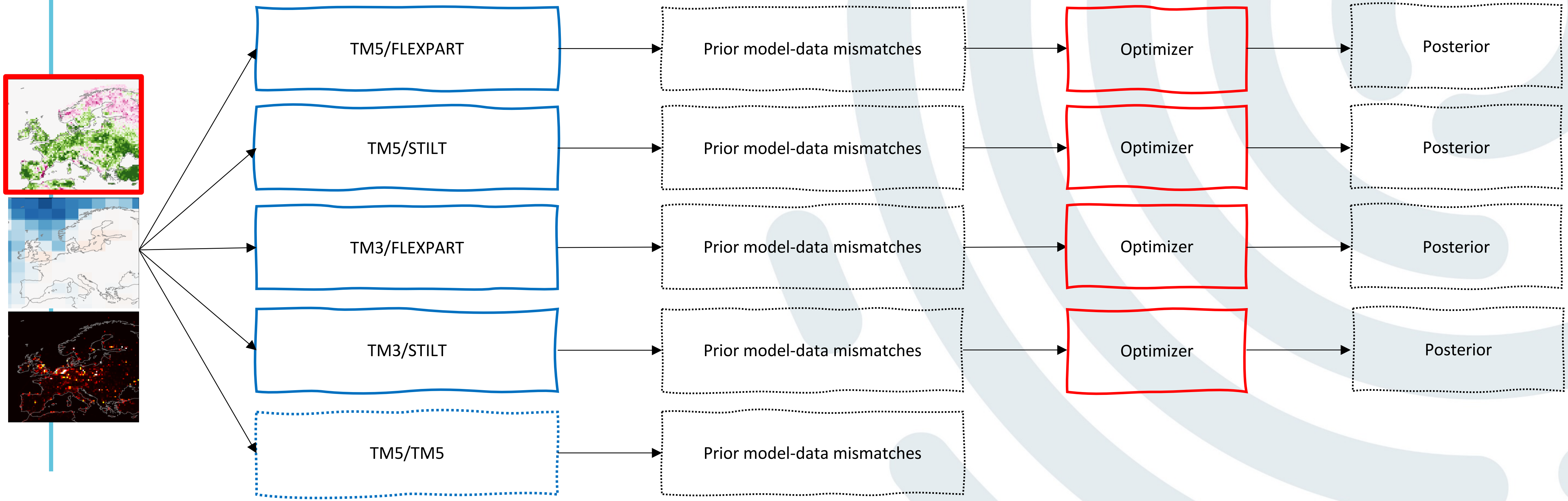
Monteil et al., ACP, 2020

	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015	Mean	SD
PYVAR-CHIMERE	0.12	0.29	0.34	0.02	0.24	0.53	0.51	0.47	0.27	0.05	0.28	0.18
CTE	-0.16	-0.01	-0.12	0.09	0.28	-0.01	0.25	-0.12	0.14	-0.10	0.02	0.16
FLEXINVERT	-0.13	-0.23	-0.19	-1.01	-0.47	-0.45	-0.34	-0.08	-0.96	-0.23	-0.41	0.33
LUMIA	-0.40	-0.36	-0.31	-0.54	-0.26	-0.24	-0.20	-0.36	-0.47	-0.45	-0.36	0.11
NAME-HB						0.09	0.35	0.40	0.07	0.17	0.22	0.15
CarboScope-regional	-0.69	-0.27	-0.04	-0.42	0.00	-0.36	-0.16	-0.29	-0.34	-0.65	-0.32	0.23
LPJ-GUESS	-0.23	-0.45	-0.46	-0.39	-0.42	-0.34	-0.09	-0.33	-0.57	-0.33	-0.36	0.13
ORCHIDEE	-0.24	-0.19	-0.22	-0.31	-0.30	-0.29	0.02	-0.26	-0.42	-0.09	-0.23	0.12
SiBCASA	-0.04	-0.08	0.01	-0.15	-0.06	-0.21	-0.02	-0.12	-0.11	-0.12	-0.09	0.07
VPRM	-0.99	-1.16	-1.11	-1.15	-1.05	-1.37	-1.01	-1.24	-1.35	-1.03	-1.15	0.14
Median posteriors	-0.16	-0.23	-0.12	-0.42	0.00	-0.13	0.05	-0.10	-0.13	-0.16	-0.15	0.17
Median priors	-0.23	-0.32	-0.34	-0.35	-0.36	-0.31	-0.06	-0.30	-0.49	-0.23	-0.29	0.13

Task 5.6: Uncertainties in European inversions of CO_2 and CH_4

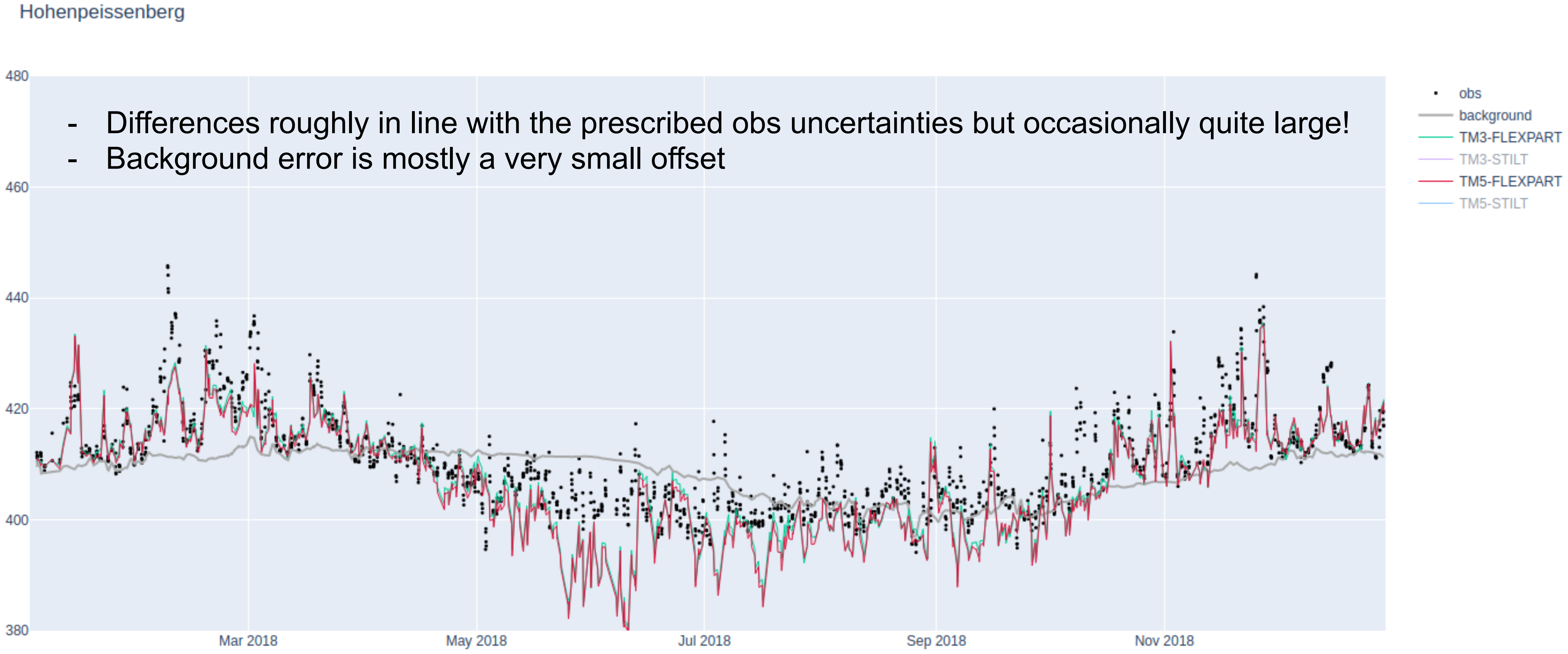
CO_2 inversions with several transport models & inversion set-ups

- Two regional Lagrangian transport models: FLEXPART and STILT (Bonus: a “regionalized” TM5 run)
- Two sets of “background” concentrations, from TM5-4DVAR and CarboScope (TM3)
- Two systems: LUMIA and Carboscope-regional



Task 5.6: Uncertainties in European inversions of CO_2 and CH_4

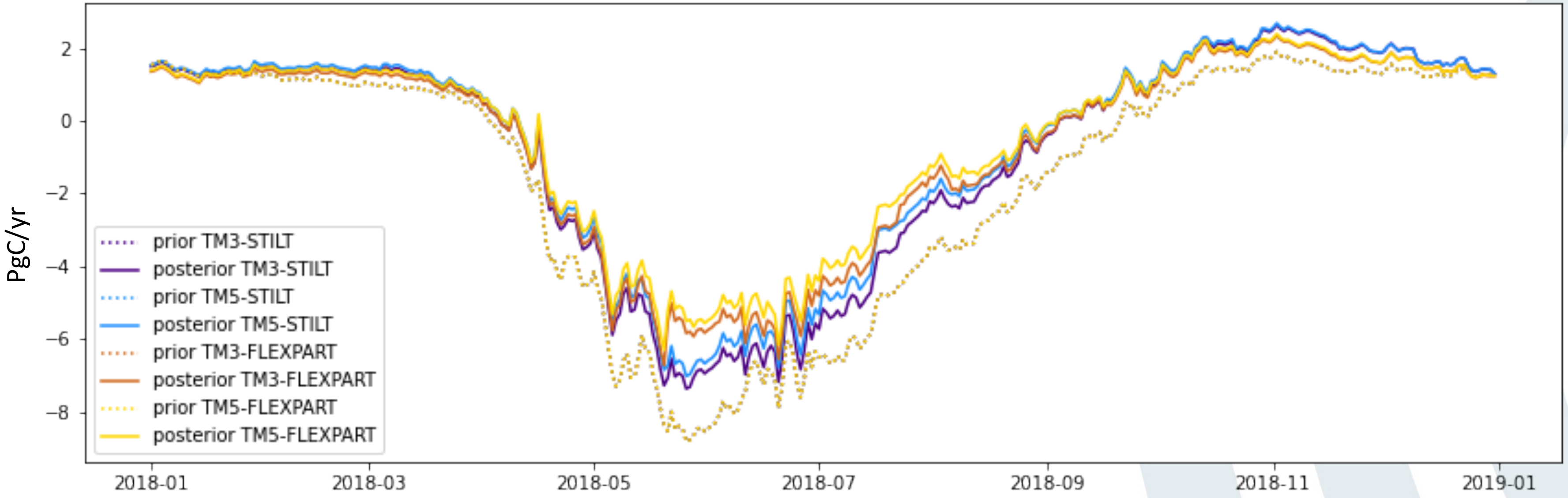
Prior model-data mismatches

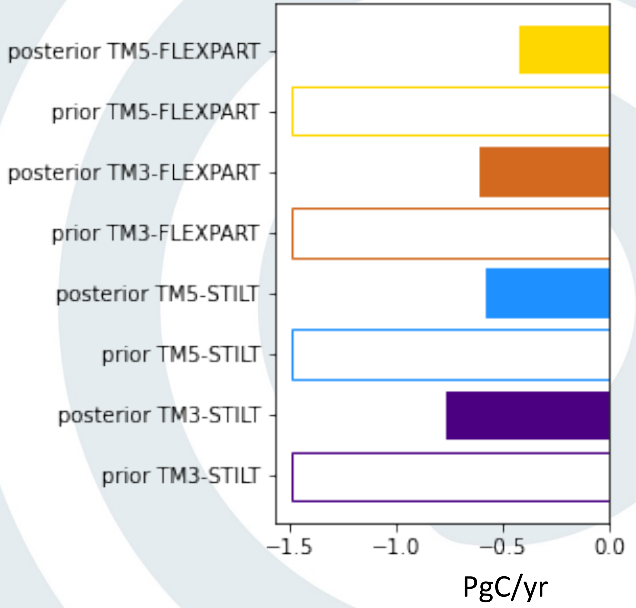


- Differences roughly in line with the prescribed obs uncertainties but occasionally quite large!
- Background error is mostly a very small offset

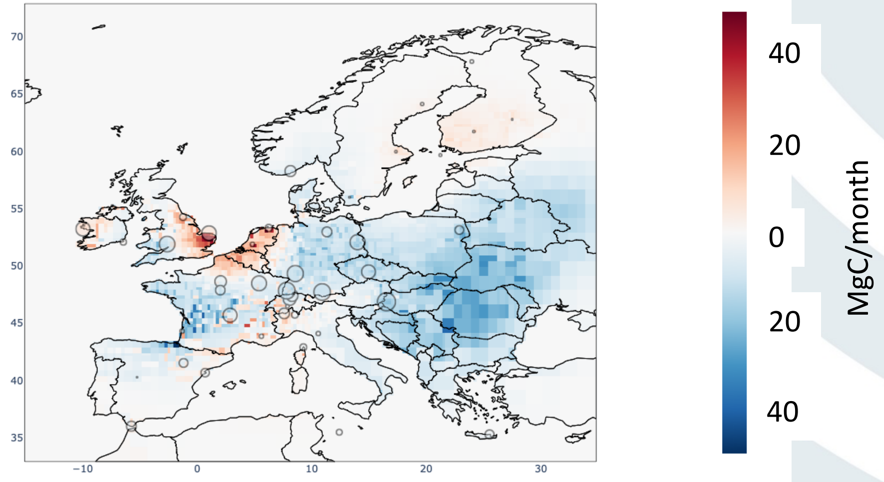
Task 5.6: Uncertainties in European inversions of CO_2 and CH_4

Posterior Fluxes





Difference FLEXPART-STILT
June 2018



Task 5.6: Uncertainties in European inversions of CO_2 and CH_4

Benchmarking methodologies & best practices for inversion-based national CH_4 emission estimates

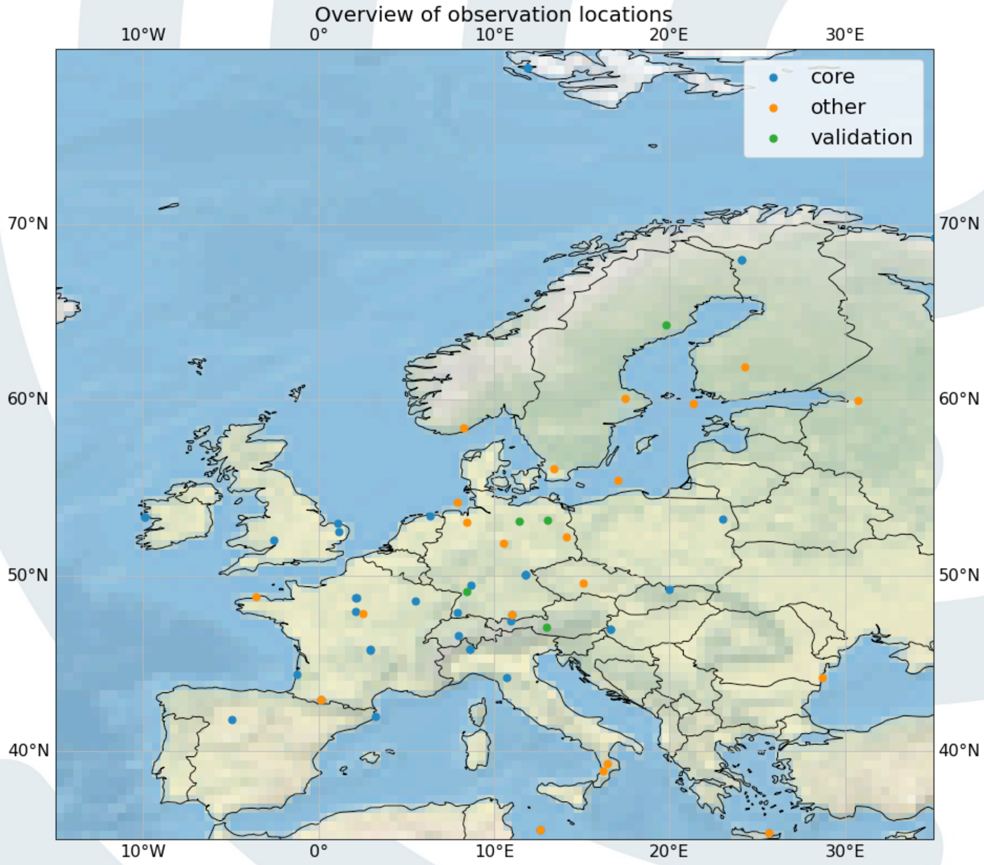
Intercomparison with 2 phases:

1. National CH_4 emissions from in situ observations (2005-2018) (Collaboration with VERIFY)
2. Extension to 2021 and addition of satellite observations

- Prior fluxes: monthly, 0.25 deg
- B.C.: CAMS reanalysis (consistent baseline fluxes for Rödenbeck 2-step approach available)
- Runs with core obs only, and inclusive

Output (core years = 2008, 2013, 2018):

- Gridded fluxes: monthly, 0.25 deg
- National total emissions and uncertainties per category
- Mixing ratios
- Radon transport



→ Contact Sander or Liesbeth for protocol

Connection with other WPs

- **WP2 (Prior and Ancillary information):**
  - Spatial explicit uncertainty information
- **WP3 (Development of global modelling and data assimilation capacity in an MWS)**:
  - WP5 benchmarking, uncertainty assessment satellite data & biospheric fluxes
  - Link between local & global system
- **WP4 (Local and regional modelling and data assimilation)**:
  - Guidance in model uncertainty
  - Link between local & global system
  - Provision of boundary conditions
- **WP6 (Integration, testing, application and initial validation of prototype systems)**:
  - Integration of information collected in WP5 in prototype CO2MVS
  - Evaluation and quality Control (EQV) tool for the CO2MVS
- **WP7 (Observations):**
  - Observational requirements EC flux, surface & satellite measurements

CoCO2

Prototype system for a Copernicus CO_2 service

THANK YOU

This presentation reflects the views only of the author, and the Commission cannot be held responsible for any use which may be made of the information contained therein.

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