



Empa

Materials Science and Technology



Status T4.3.4: Very high-resolution inversions

**Dominik Brunner¹, Peter Bergamaschi², Arjo Segers³
and Jean-Matthieu Haussaire¹**

¹Laboratory for Air Pollution/Environmental Technology, Empa, Dübendorf, Switzerland

²European Commission Joint Research Centre, Ispra, Italy

³TNO, Climate, Air and Sustainability, Utrecht, the Netherlands

Development and application of a very high resolution inversion system

- Based on atmospheric transport simulations with FLEXPART-COSMO driven by hourly meteorological analysis fields of COSMO at 7 km x 7 km resolution
- Estimation of European CH₄ and N₂O emissions at 0.125° x 0.125° spatial and weekly temporal resolution
- Minimization of cost function with 4D-VAR approach
- Nesting into global TM5-4DVAR system using two-step approach of Rödenbeck et al. 2009
- Comparison with Extended KF and regular VERIFY inversion

**Final product: 0.06° x 0.06° spatial
& monthly temporal resolution**

Deliverable D4.15 (due month 42)

CH₄ flux maps at 0.125°x0.125° for Western/Central Europe for 2010-2015

- 4-DVAR: Computation of gradient of cost function $\nabla_x J = B^{-T/2}(x - x_b) + H(x)^T R^{-1}(H(x) - y)$ and minimization using M1QN3 or CONGRAD algorithm
- State transformation (pre-conditioning) for better convergence
- Background from global TM5-4DVAR run following two-step approach of Rödenbeck et al. (2009)

Further design aspects:

- Precise embedding of the non-rectangular domain of FLEXPART-COSMO into TM5-4DVAR
- Precise mapping of a priori fields onto the rotated-pole grid of FLEXPART-COSMO
- Careful consideration of model representation errors (e.g. based on meteorology)
- Optimization of parameters (amplitude, correlation length scales) of prior and observation covariance matrices with a maximum-likelihood approach

Main developers: Arjo Segers (TNO) & Peter Bergamaschi (JRC)

- Sequential assimilation of observations (daily updates)

$$\mathbf{x}_k^+ = \mathbf{x}_k^- + \mathbf{K}_k \cdot (\mathbf{y}_k - \mathbf{H}_k \mathbf{x}_k^-),$$

- Optimization of logarithm of emissions, $x = \ln(e)$, to ensure positive solution and normally distributed residuals
- Error growth possible due to forecast step

$$\mathbf{x}_k^- = \mathbf{x}_{k-1}^+ + \boldsymbol{\eta}_k$$

- Reduced grid with lower resolution where coverage (sensitivity) of measurement network is lower
- Same background as for FLEXVAR (Rödenbeck two-step approach)

- Driven by hourly meteo fields from COSMO at 7 km x 7 km resolution
- Simulations for 54 stations, partly with multiple release heights
- 50'000 particles released every 3 hours and followed backwards over 10 days (results presented here still based on 4 day bkwd simulations)
- Particle residence times (footprints) stored at 7 km x 7 km resolution
- Positions and times of particles stored when they leave domain or are terminated

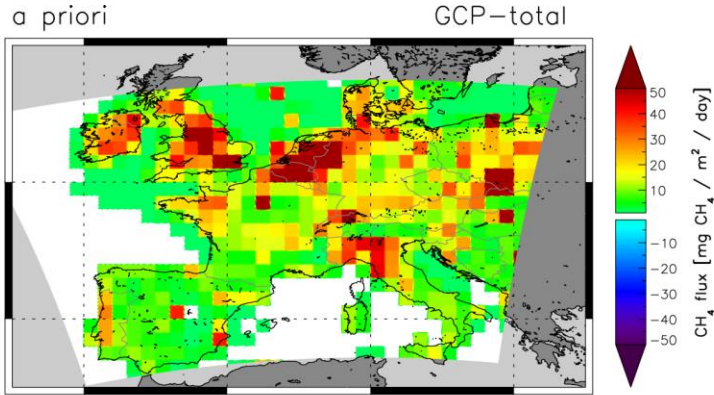
Observations

- Core sites: ICOS release 2019-1 (13 sites)+ NOAA flask sampling (5 sites)
- Extended: Core + UK sites (BSD, TAC, RGL, HEA, WAO) + AGAGE (MHD) + TNO (CBW) + LSCE (BIS) + U. Bern/Empa (BRM, LAE) + ??

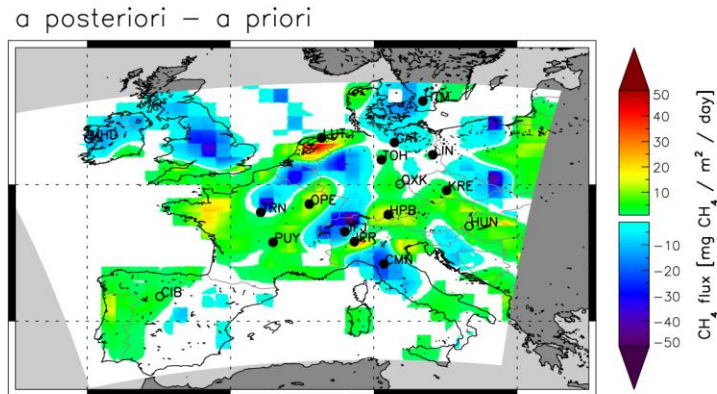
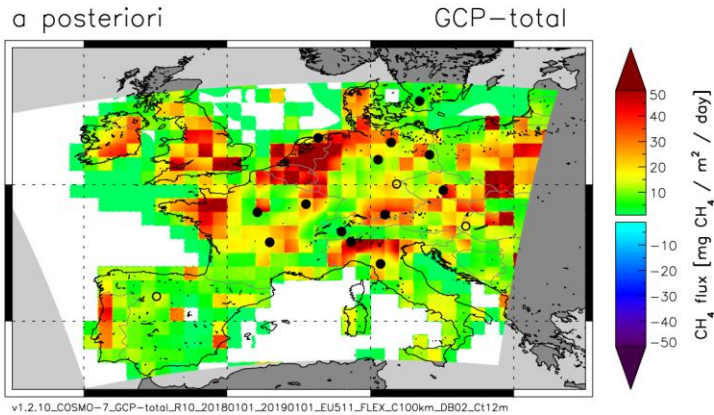
Prior fluxes

Source	Model/Reference	Resolution/coverage
Anthropogenic	GCP-2018, EDGAR-v4.3.2	Global 1°×1°, monthly (2017)
Wetlands	GCP-2018, Poulter et al.	Global 1°×1°, monthly, climatology
Biomass burning	GFEDv4.1s + EDGAR FFF&RCO	Global 1°×1°, monthly
Ocean	GCP-2018, Lambert et al.	Global 1°×1° annual, climatology
Termites	GCP-2018, Castaldi et al.	Global 1°×1° annual, climatology
Geological	GCP-2018, Etiope book	Global 1°×1° monthly

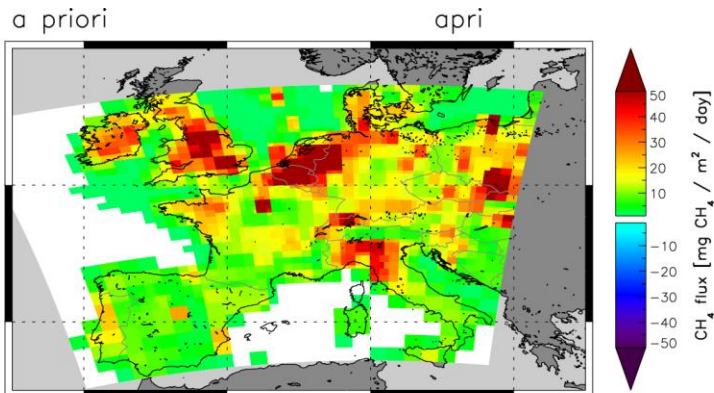
Comparison between FlexVar and FlexKF



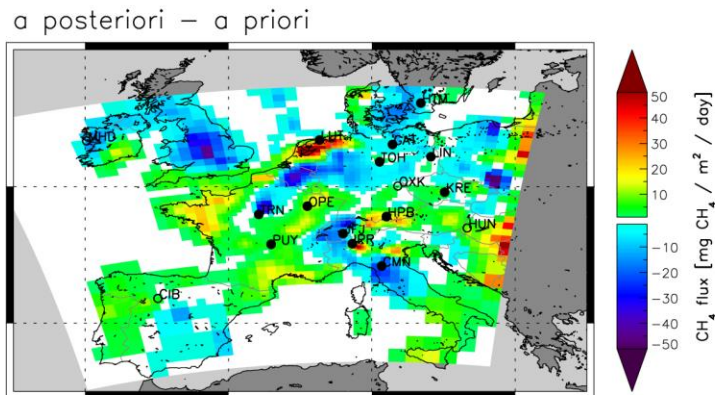
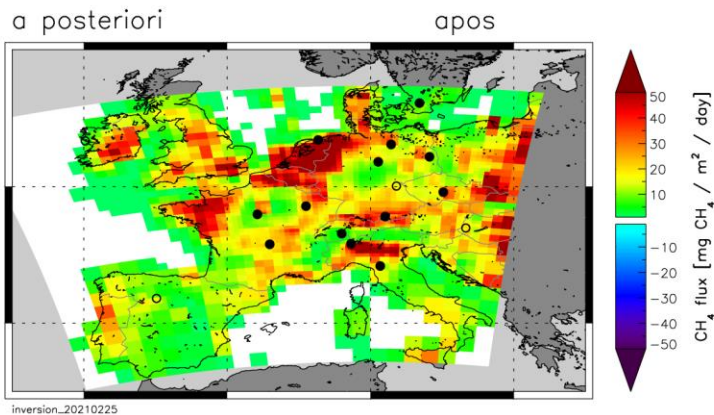
FlexVar annual mean 2018



Comparison between FlexVar and FlexKF



FlexKF annual mean 2018



Inversion_20210225

Influence of baseline and station release heights

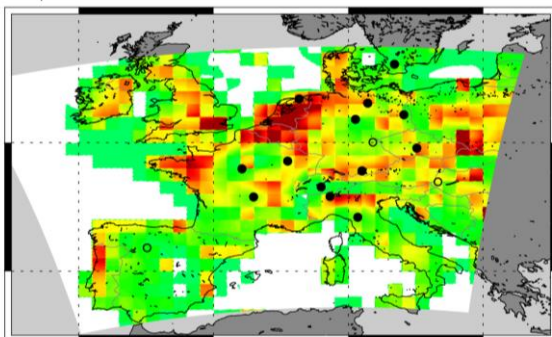


Baseline treatment

Example for FLEXVAR

Rödenbeck scheme

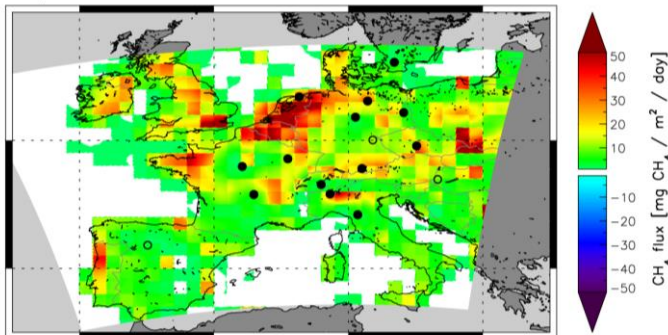
a posteriori GCP-total



v1.2.11_COSMO-7_GCP-total_R03_20180101_20190101_EU511_C100km_C12m_OL

Particle dumps

a posteriori GCP-total



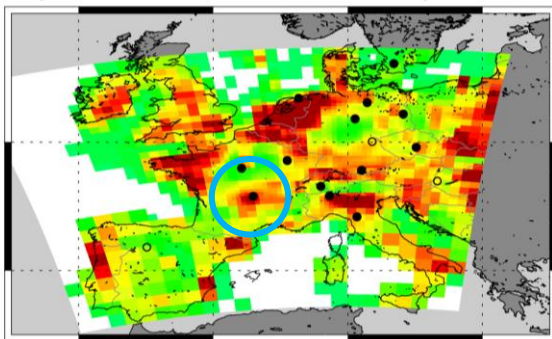
v1.2.11_COSMO-7_GCP-total_R03_20180101_20190101_EU511_C100km_C12m_m.p_OL

Release height

Example for FlexKF

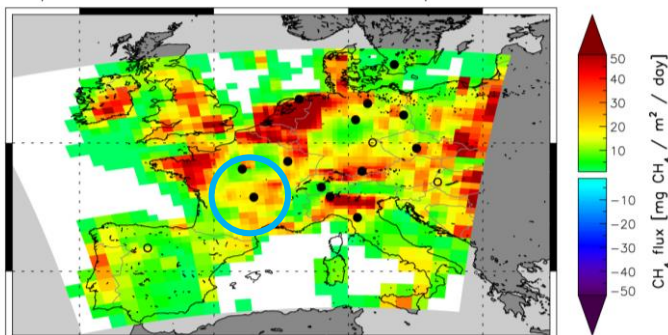
True station height

a posteriori apos



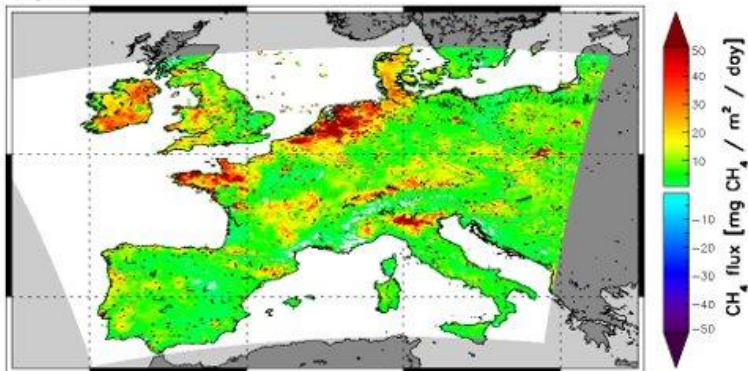
Optimal height

a posteriori apos



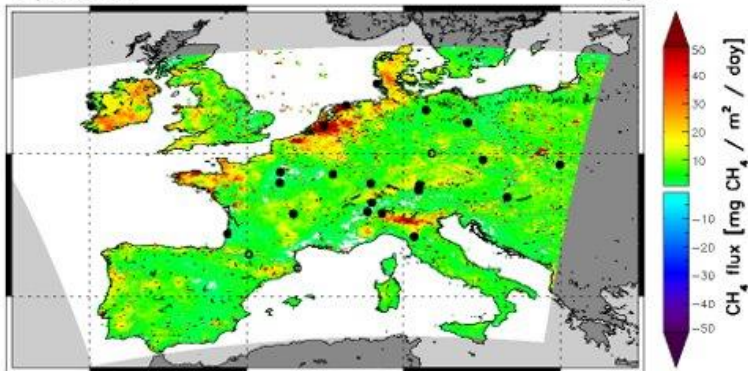
Example of high-resolution inversion for 2017

a priori



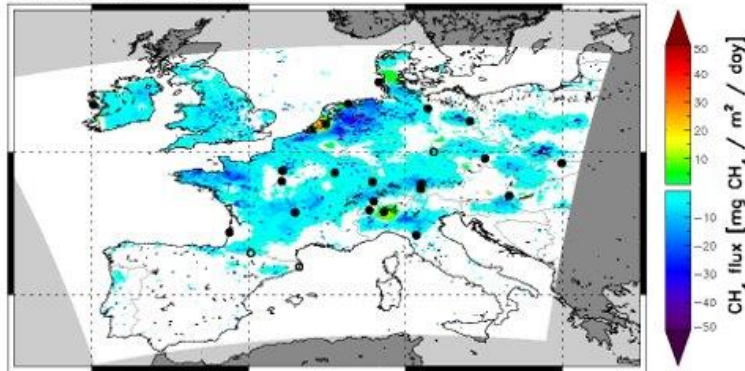
A priori:
EDGAR 5.0, 0.1° x 0.1° resolution
(no natural sources)

a posteriori



apos

a posteriori – a priori



apos

v1.2.2.0594D-7_MAR2022_VERIFY_20170101_20180101_LEU5IS_FLEX_S02_160

- FLEXVAR system fully functional: sophisticated, flexible and well-documented 4D-VAR inversion tool
- Coupled global (TM5-4DVAR) – regional (FLEXPART-COSMO) inversion implemented using two-step Rödenbeck approach
- First inversions performed for 2018 with ICOS + NOAA flask sites only and with coarse a priori (for consistency with global TM5-4DVAR)
- FLEXVAR allows optimizing state vector with $O(10^5)$ elements
- Comparison with FlexKF shows largely consistent results, except for domain boundaries where FlexKF shows stronger adjustments
- 4-day backward simulations not enough for Rödenbeck scheme -> new 10 days
- Choice of particle release height for mountain sites has strong impact on results