

1. Introduction

The CHIMERE air quality model has been implemented into the Data Assimilation Research Test bed system (DART) from the National Center Atmospheric Research for regional data assimilation application over Europe. The Ensemble Adjustment Kalman Filter (EAKF) is currently applied at INERIS to perform analysis based on EEA surface observations. The ability to assimilate Vertical Column Density (VCD) of SENTINEL 5P Satellite TROPOMI (Retrieval S5P, L2 products) of various chemical species are now studied within the framework of the CAMs EvOluTion project (CAMEO : <https://www.cameo-project.eu/>, 36 months project from 01/2023 to 12/2025) coordinated by ECMWF. Performing high resolution analysis at regional scale using both surface observations and satellite data remains a challenge for air quality applications. Chemical processes can be complex and strongly nonlinear, involve a large number of species and costly to solve in CPU time. We show work in progress for NO₂ and SO₂ DA and issues that need to be addressed.

2. Setup & Method

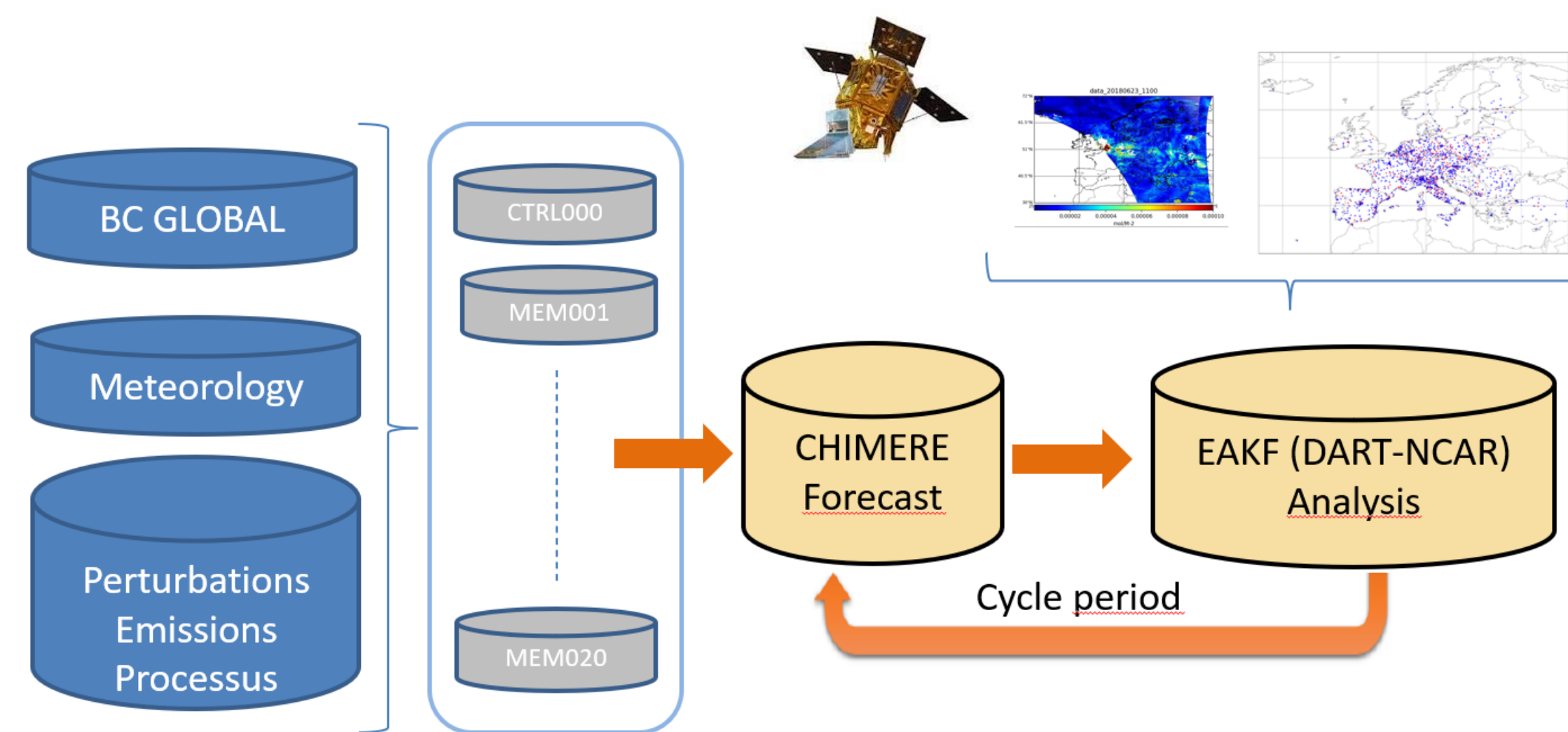


Fig 1 : CHIMERE-DART EAKF configuration over Europe to assimilate surface observations and satellite data at high resolution.

- Model configuration: CHIMERE CTM is driven by IFS model (ECMWF) for the meteorology and the boundary conditions. Anthropogenic emissions come from CAMS-REG inventories (2018 & 2022). The horizontal resolution of CHIMERE is 0.2 degree. The operational configuration of 9 vertical levels simulation with at top at 500 hPa has been extended to 20 vertical levels with a top 200 hPa.
- Ensemble DA: 21 members coming from perturbations on emissions, meteorology, deposition and photolysis rates. Gaspari-Cohn (GC) fifth-order rational function [Gaspari and Cohn, 1999] error covariance localization is done to avoid spurious long-range correlation due to finite ensemble size. Prior inflation.
- Observations:
 - AIRBASE reporting surface observation concentration (hourly). Dataset splitted for DA and validation purpose (blue/red dots Fig 1 for NO₂).
 - The TROPospheric Monitoring Instrument (TROPOMI) instrument on board the Copernicus Sentinel-5 Precursor satellite has a near-polar, sun-synchronous orbit, an improved ground pixel size of 5.5 km × 3.5 km since 2019 and swath width about 2600 km. (UV-VIS NO₂ & SO₂).

3. Results of NO₂ satellite DA

Comparison on the period March 2020 of NO₂ RS5P DA using only satellite data experiments (RS5Ponly) with satellite data and surface observations DA experiment (RS5Psurf)

Observation space

- Increment mainly positive due to strong underestimation of NO₂ in CHIMERE.
- Largest corrections are located around big cities such as Istanbul, Alger, Po valley.
- Increment can be locally negative such as in the region of Anvers/Rotterdam, close to the eastern border of Germany, and in the center of Poland.

NO₂ surface concentration

- Common patterns in the increments : stronger positive increment for middle and the southern european countries. Negative increment in Netherland (Fig 3).

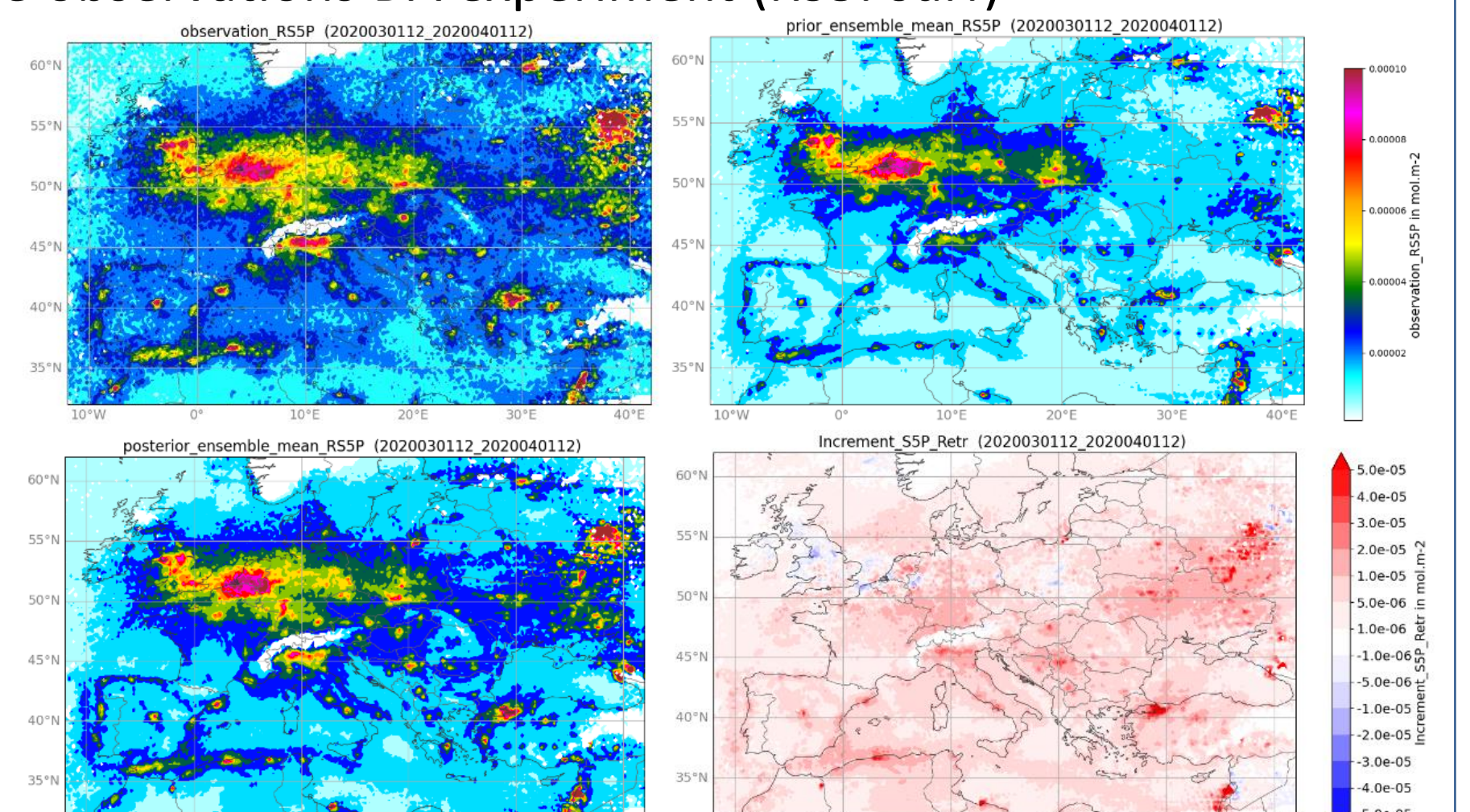


Fig 2 : NO₂ Retrieval SENTINEL 5P data (top left), CHIMERE observation operator ensemble mean prior/posterior (top right/bottom left), increment (bottom right).

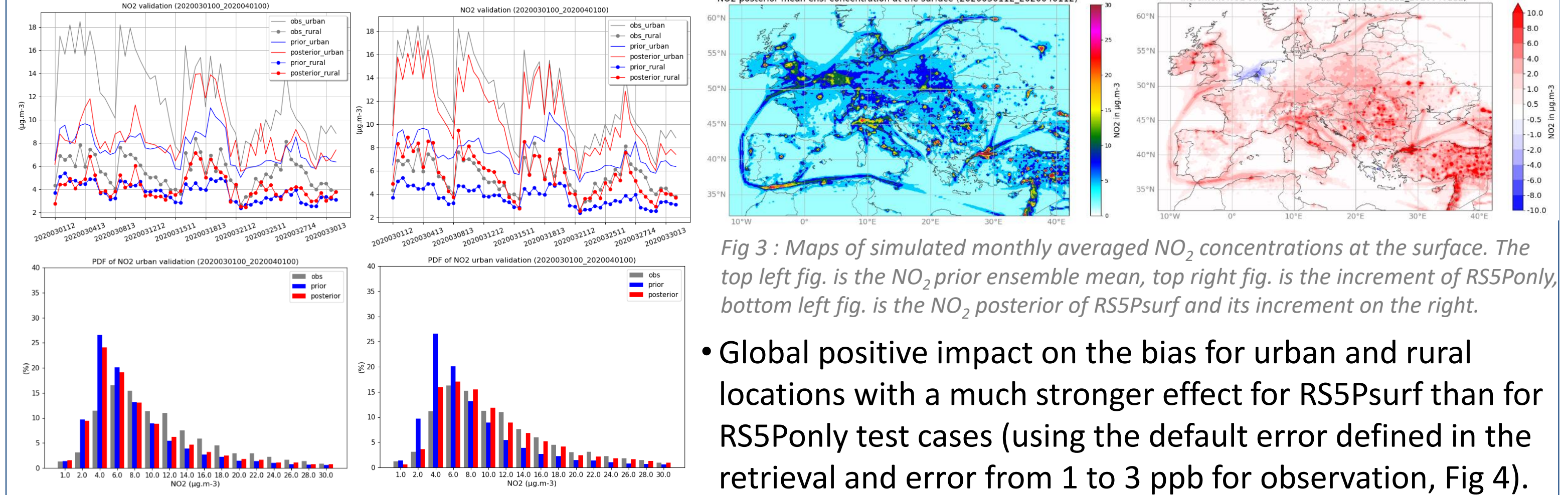


Fig 3 : Maps of simulated monthly averaged NO₂ concentrations at the surface. The top left fig. is the NO₂ prior ensemble mean, top right fig. is the increment of RS5Ponly, bottom left fig. is the NO₂ posterior of RS5Psurf and its increment on the right.

Fig 4 : Surface NO₂ concentrations interpolated and averaged at observation locations on top, PDFs for urban site at the bottom. RS5Ponly on the left, RS5Psurf on the right.

- Global positive impact on the bias for urban and rural locations with a much stronger effect for RS5Psurf than for RS5Ponly test cases (using the default error defined in the retrieval and error from 1 to 3 ppb for observation, Fig 4).
- Decrease in % of the lowest concentrations and an increase in % of the highest concentrations (PDFs).

4. Future work

DA of TROPOMI SENTINEL S5P columns for SO₂, CO, O₃ and HCHO.

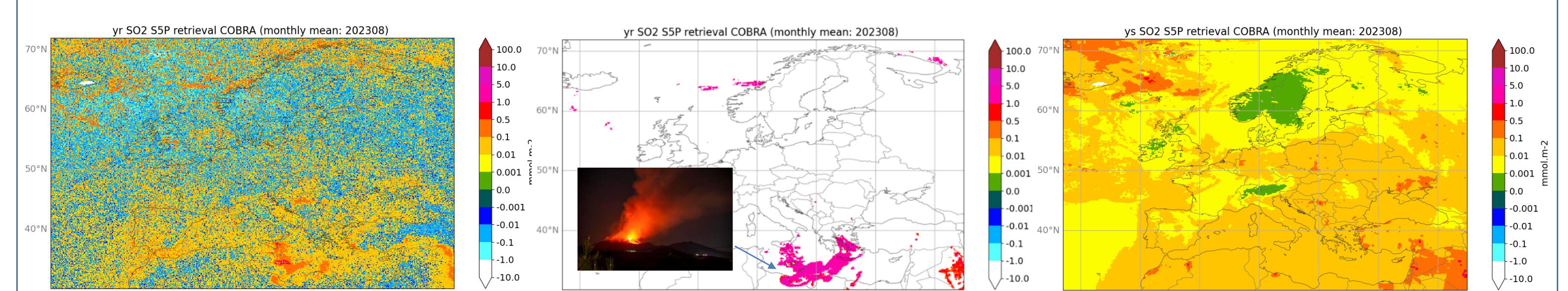


Fig 5 : Comparison of monthly average SENTINEL 5P SO₂ columns, in the left fig. S5P-COBRA retrievals regridded to 10 km, in the middle fig. S5P-COBRA, only clear detection close to known anthropogenic source and volcano and in the right fig. CHIMERE obs. operator.

- Raw data may still be noisy for monthly averaged. Negative retrieval values can be found in the nordic countries and over the Alps mountains where the lowest values of CHIMERE are found.
- High polluted area such as in Serbia, Türkiye can be identified.
- No SO₂ plume in average representing the volcano ETNA eruption in operational CHIMERE. Work in progress to improve the background error using tagging (SO₂ volcanic) and reduce chemical mechanism SO₂. Benefit of increasing the number of members with low CPU cost.
- Performing emissions inversion : benefit in the forecast (SO₂, HCHO, CO).
- Test advanced DA methods (non gaussian), Kalman smoother, small ensemble.
- Satellite bias correction most likely need to be addressed.

5. Conclusions

- The comparison of DA experiment of SENTINEL 5P VCD of NO₂, RS5Ponly with RS5Psurf experiment, shows similar patterns and tendencies in the analysis. More benefits of using RS5Ponly of NO₂ most likely when no dense surface observation network is available. Continue working on for better co-assimilation of RS5P and surface observations. Going from Polar orbiting SENTINEL 5P to SENTINEL 4 geostationary satellite within NO₂ OSSE in Task 3.3 in CAMEO.
- Comparison of different DA approaches in Task 3.1 CAMEO for DA of TROPOMI SENTINEL S5P products. (INERIS, FMI, AU, ENEA, FZJ, SMHI, IOS-PIB).

Contact us

Gael Descombes
 INERIS
 Email: gael.descombes@ineris.fr
 Website: <https://www.ineris.fr>
 Phone: 03-44-55-66-77

References

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