ITALIAN NATIONAL AGENCY FOR
NEW TECHNOLOGIES, ENERGY AND
SUSTAINABLE ECONOMIC DEVELOPMENT

Assimilation of atmospheric constituents provided by satellite data with Optimal Interpolation and DART-EnAKF implemented in Atmospheric Modelling System MINNI

M. MIRCEA[1], A. BOLIGNANO[1], M. ADANI[1], G. BRIGANTI[1], F. RUSSO[1], A. D'AUSILIO[2], G. DE MOLINER[3], C. SILIBELLO[2]

[1] Italian National Agency for New Technologies, Energy and Sustainable Economic Development (ENEA), Via Martiri di Monte Sole 4, 40129 Bologna, Italy
[2] ARIANET srl, 20159 Milano, Via Benigno Crespi 52, Italy.
[3] Department of Civil and Environmental Engineering, Politecnico di Milano, Piazza Leonardo da Vinci 32, Milan, 20133, Italy

AOC-CLIMAR-SSPT, ENEA

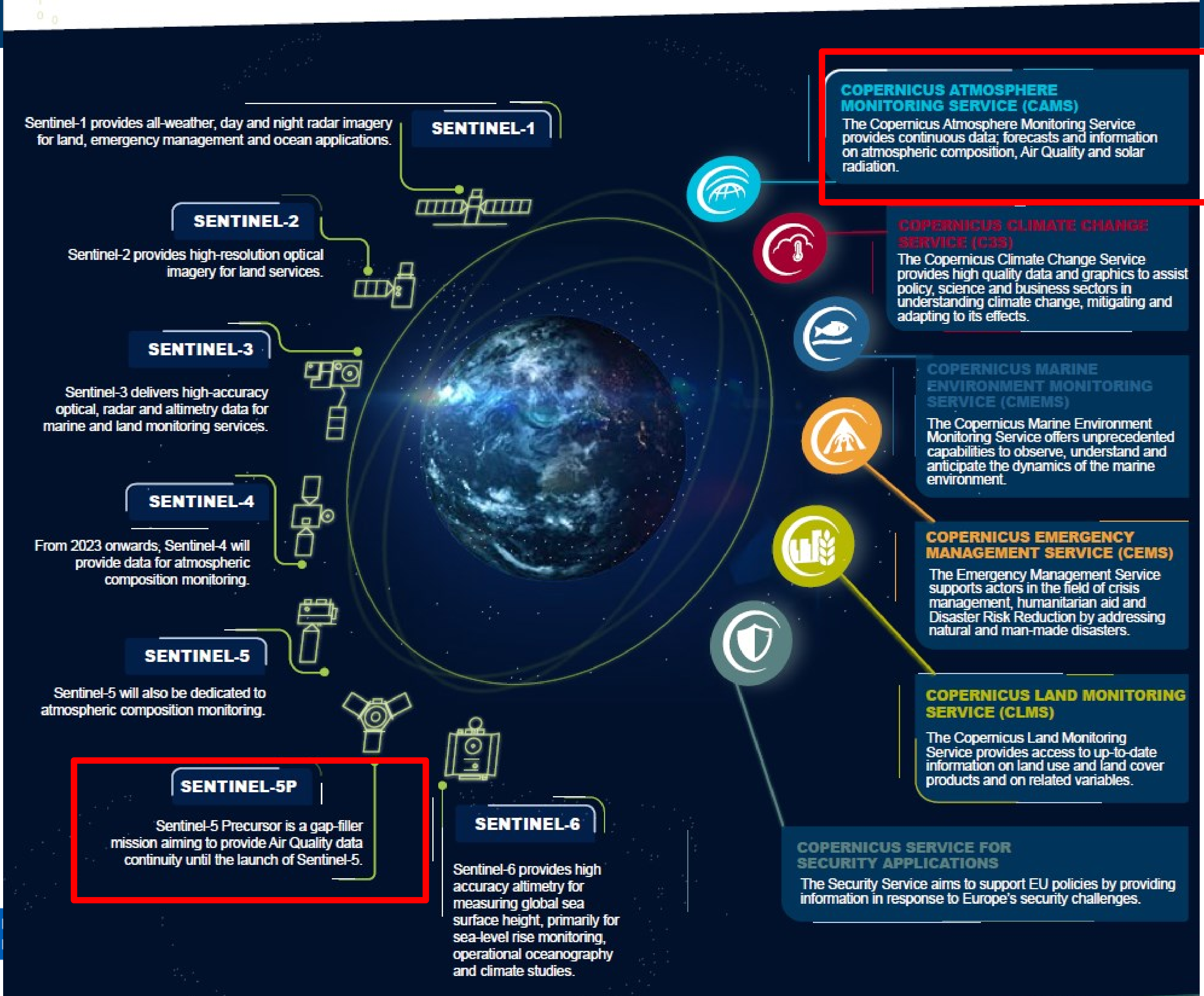
Bologna, 20 marzo 2025

Satellite Data: Europe and U.S.A

"The **U.S.** National Oceanic and Atmospheric Administration (NOAA) has a long history of satellite observations, including for atmospheric composition. Stratospheric ozone measurements have been made by **NOAA since the 1980s**, and over the years, NOAA's weather satellites have added other atmospheric composition capabilities, particularly **volcanic ash, dust, smoke aerosols, and limited tropospheric trace gas measurements** (e.g., Zhang et al. 2022; Nalli et al. 2020; Shephard et al. 2020; Wells et al. 2022; Li et al. 2015). These products already support a number of applications, especially timely information about aerosols and wildfire smoke observations provided through AerosolWatch. Expanding its spaceborne atmospheric composition focus, NOAA has made plans for a dedicated ultraviolet–visible (UV–Vis) instrument aboard its next-generation geostationary constellation, GeoXO, expected to launch in the 2030s. As NOAA begins planning for the next generation of low-Earth-orbit (LEO) satellites, it is users' input on the needs for LEO satellite data in the 2040s and beyond, when NOAA's current operational Joint Polar Satellite System (JPSS) series of satellites will reach end of life." (https://doi.org/10.1175/BAMS-D-22-0266.1)

SIX THEMATIC SERVICES

— The Copernicus component of the EU Space Programme also includes six thematic services that allow public and private users to use Copernicus data to tackle a wide range of societal challenges.



Sentinel-5P: TROPOMI

Image Credit/Copyright: ESA/ATG medialab

The Copernicus Sentinel-5 Precursor mission reduces gaps in the availability of global atmospheric data products between SCIAMACHY/Envisat (which ended in April 2012), the OMI/AURA mission and the future Copernicus Sentinel-4 and Sentinel-5 missions.

- Sentinel-5 Precursor
- Low Earth Orbit Atmospheric Chemistry Mission
- Launched -13 October 2017 by ESA
- The TROPOMI instrument is UV-VIS-NIR-SWIR push-broom grating spectrometer.c, it is based on the DOAS technique, the most widely used method to derive atmospheric trace gas constituents in the UV–visible spectral range.

- The S5p sensor TROPOMI samples the Earth's surface with a revisit time of one day and with aspatial resolution of 7.0x3.5 km2 , respectively 5.5×3.5km2 (since 6th of August 2019)

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(https://sentiwiki.copernicus.eu)

TROPOMI is a key data contributor for Copernicus Atmosphere Monitoring Service (**CAMS**) and Copernicus Climate Change Service (**C3S**)

instrument	*satellite*	*swath width*	*ground pixel size*
GOME-1	ERS-2	960 km	320 x 40 km
SCIAMACHY	ENVISAT	960 km	60 x 40 km
OMI	EOS-AURA	2600 km	12 x 24 km
GOME-2	MetOp-A	1920 km	80 x 40 km

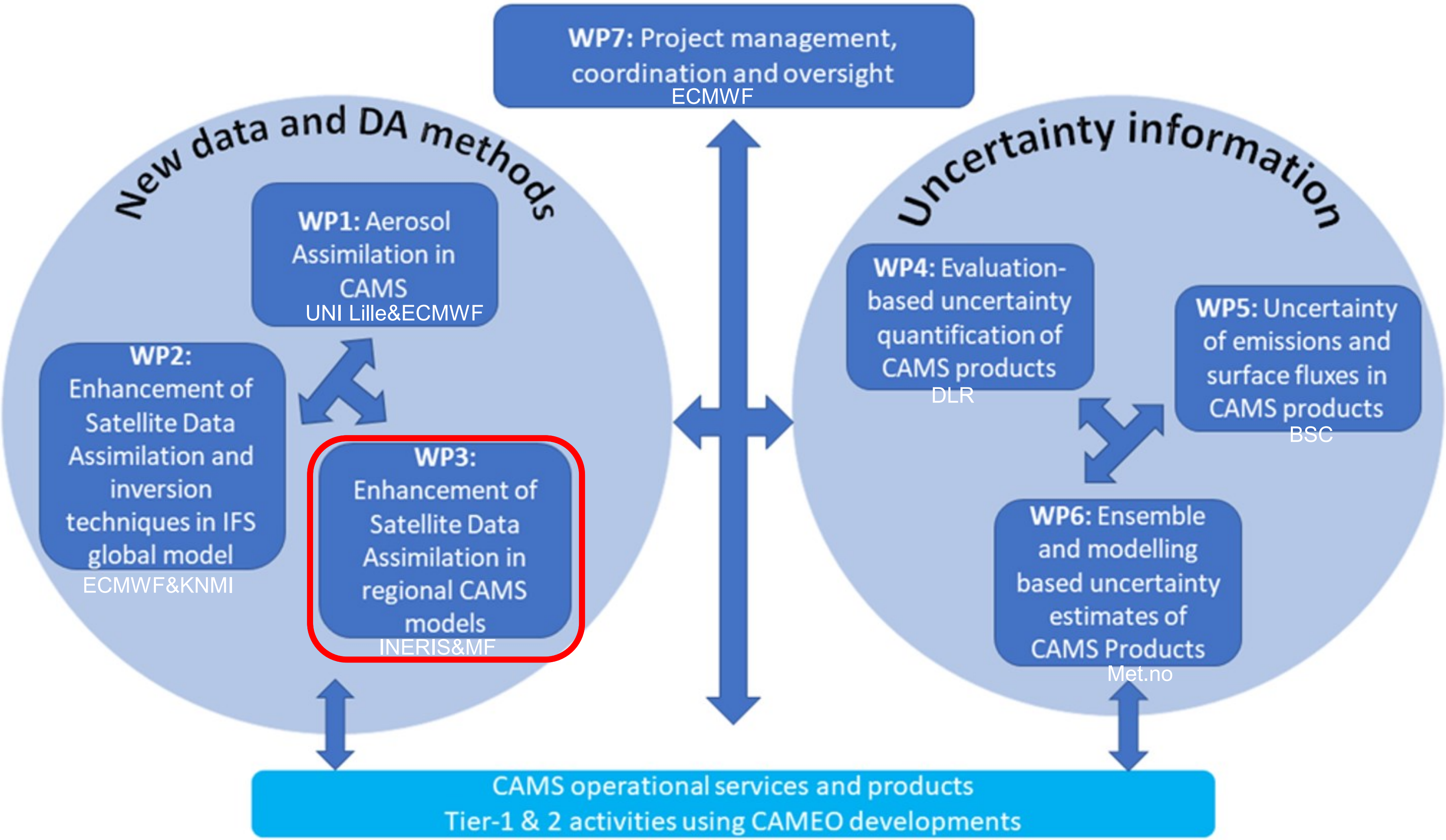
ENEA

Sentinel-5P products

Application	Sentinel - 5P Product type										
	O3	O3_TCL	03_PR	NO2	SO2	CO	CH4	HCHO	CLOUD/ NP_BDx	AER_AI	AER_LH
Air Quality & Pollution	✔	✔		✔	✔	✔	✔	✔		✔	✔
Climate Change	✔	✔		✔	✔	✔	✔	✔	✔		
Aviation Safety					✔					✔	✔
Ozone and Ozone Layer Control	✔	✔	✔	✔							
Support to other S5P Products									✔		

(https://sentiwiki.copernicus.eu)

CAMEO (CAMs EvOlution)
www.cameo-project.eu



CAMEO – WP3 Enhancement of Satellite Data Assimilation in regional CAMS models
T3.1 Assimilation of Sentinel 5p TROPOMI products (INERIS, FMI, AU, ENEA, FZJ, SMHI, IOS-PIB)

- Task 3.1.1: Assimilation of TROPOMI SO2 in CAMS2_40 Regional Models. All seven teams contributing to Task 1 will assess the added value of assimilating SO2. The assessment will include a sensitivity to the choice of the selected retrieval. The development will be strongly dependent on the individual assimilation techniques in the 7 models participating in Task 1. The coordination will focus on designing consistent numerical plans in the selection of retrieval products and evaluation procedure to demonstrate the added value for the air quality system as a whole.

- Task 3.1.2: Assimilation of TROPOMI CO, O3, HCHO in CAMS2_40 Regional Models. Selected teams will assess the feasibility and added value of assimilating additional gaseous species.

Data Assimilation
-assimilation of measurements at stations-

Data assimilation refers to a large group of methods that update information from numerical computer models with information from observations. Data assimilation is used to update model states, model trajectories over time, model parameters, and combinations thereof.

(Wikipedia)

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Data assimilation experiments over Europe with the Chemical Transport Model FARM

Mario Adani [a,*], Francesco Uboldi [b,c,1]

[a] ENEA, Bologna, Italy
[b] Previous affiliation: ARIANET Srl, Milano, Italy
[c] Current affiliation: CIMA Foundation, Savona, Italy

HIGHLIGHTS

- An assimilation scheme based on 3Dvar/O.I. is implemented on CTM FARM model.
- Results are consistent with CAMS ensemble reanalysis.
- Spatial Consistency Test improves model skill scores.
- Advance quality control of assimilated observations improves model estimates.

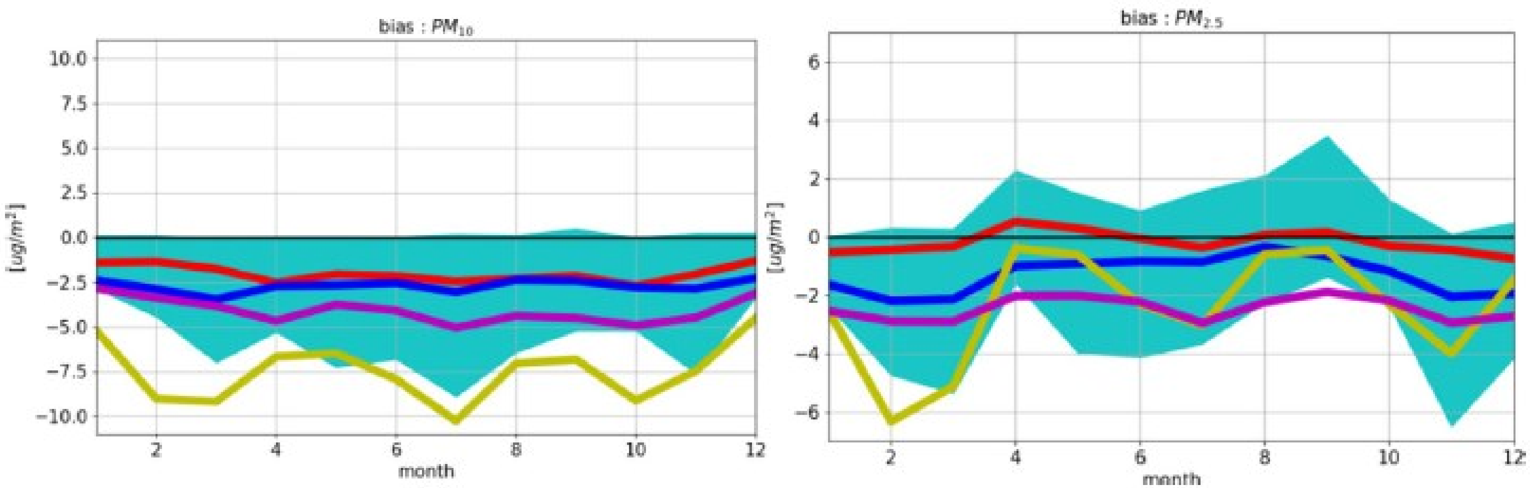
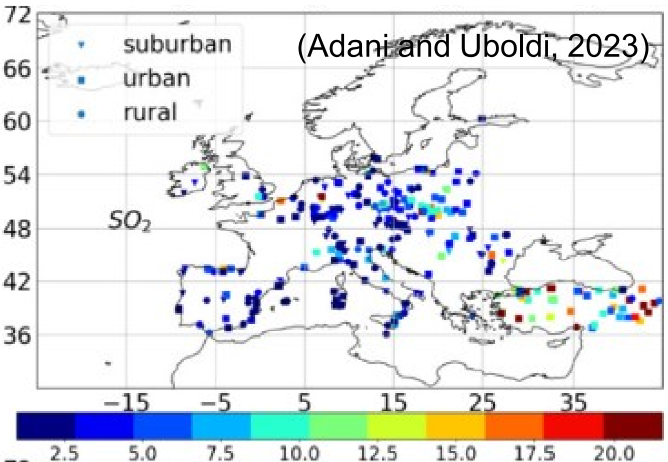
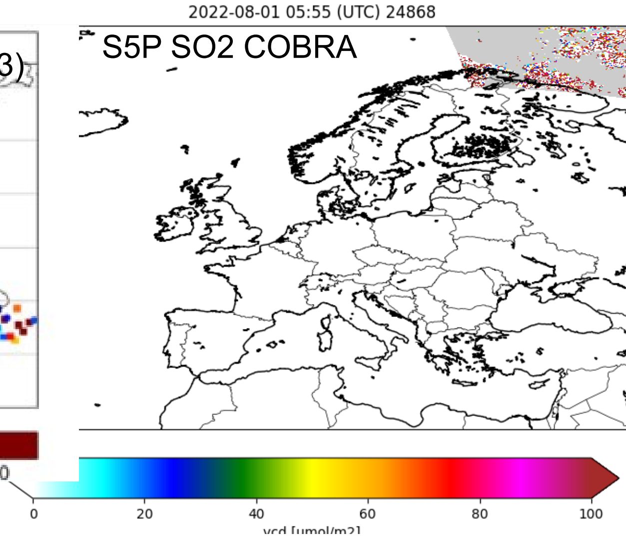
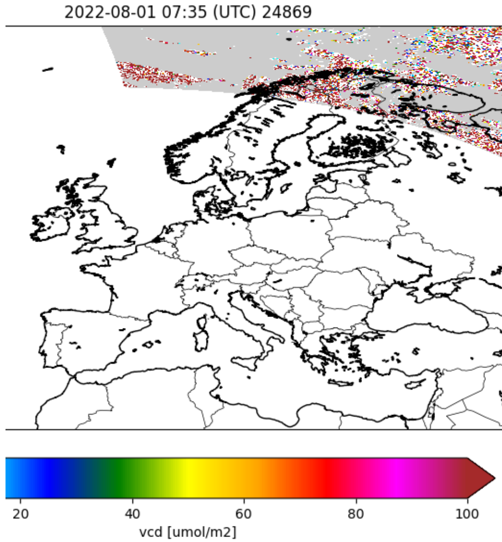


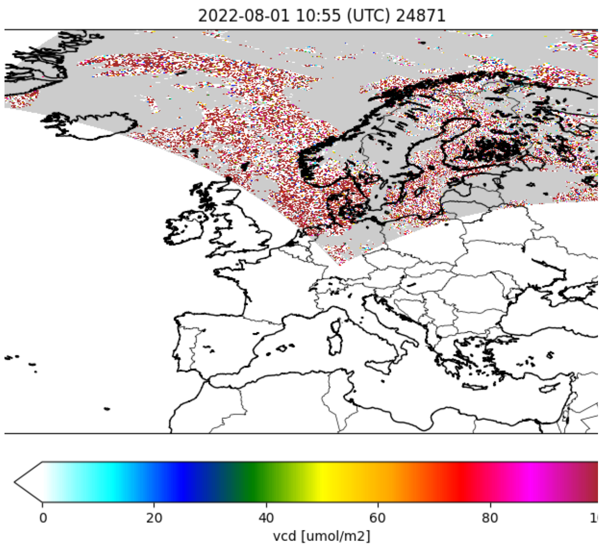
Fig. 4. Median of the monthly bias computed on station for validation. Blue line is the VRA ensemble, red is MINNI with BF and SCT, magenta MINNI with only BF, yellow is the "free run". Shaded area is the spread of CAMS members.

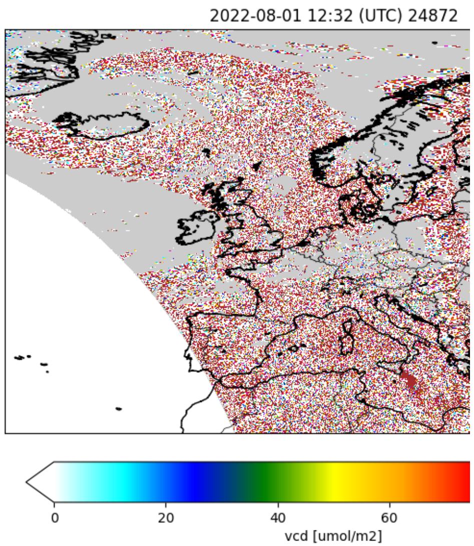
Data Assimilation
-measurements at stations and satellite data-

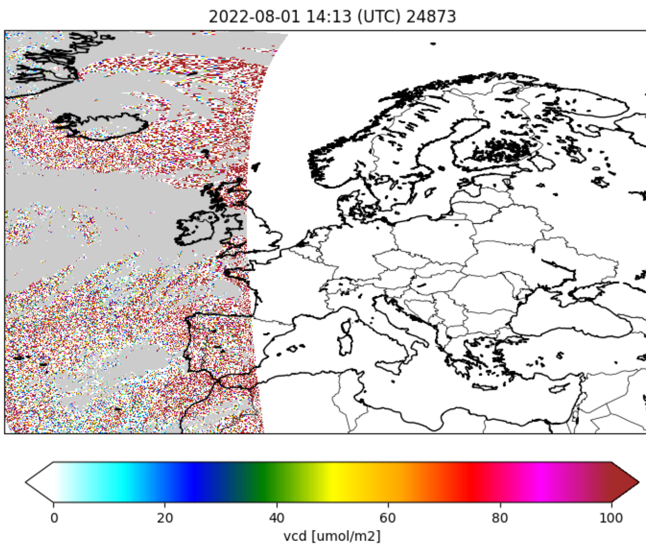












CSO - CAMS Satellite Operator

Tools for assimilation of satellite data in regional air quality model.

Aarjo Segers (https://ci.tno.nl/gitlab/cams/cso)

Observation operator SO2-COBRA (T3.1.1 CAMEO)

A model simulated column is :

$$y_s\ (x_m) = \sum_l A_l\ Hx_{m,l}$$

- x_m is the local model apriori profile
- ***A*** is the averaging kernel defined on the *a priori* layers
- ***H*** is the horizontal and vertical mapping operator from model grid to layers to *a priori* layers

- Possible benefit of using Air Mass Factor (AMF) as reported in the PUM and Duros et al 2023 (https://doi.org/10.5194/gmd-16-509-2023)

- AMF : ratio between optical thickness of vertical and slant vertical column. By default, AMF are provided with TM5 apriori profile and the user.

Alternative AMF is defined by:

$$M^*_m(x_m) = M(x_a)\sum_l A_l\ Hx_{m,l} / \sum_l Hx_{m,l}$$

- x_a is the apriori TM5 profile
- x_m is the local model apriori profile
- $M(x_a)$ is the TM5 airmass factor
- ***A*** is the averaging kernel defined on the *a priori* layers
- ***H*** is the horizontal and vertical mapping operator from model grid to layers to *a priori* layers

Courtesy of Gaël Descombes (INERIS)

Error Covariances in Data Assimilation

Error covariance matrix describes the spread and correlation of errors in a given dataset.

General Form of an Error Covariance Matrix

A covariance matrix P is given by:

$$P = \mathbb{E}[(x - \bar{x})(x - \bar{x})^T]$$

where:

- x is the estimated state vector (e.g., temperature, pressure at different locations).
- $\bar{x}$ is the mean of the state vector.
- $\mathbb{E}[\cdot]$ denotes the expectation (statistical mean).

Each element of P represents how errors in different variables are related:

$$P = \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \sigma_{13} & \cdots \\ \sigma_{21} & \sigma_2^2 & \sigma_{23} & \cdots \\ \sigma_{31} & \sigma_{32} & \sigma_3^2 & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{bmatrix}$$

where:

- σ_i^2 (diagonal elements) = **variance of errors** for state variable i (uncertainty in individual values).
- σ_{ij} (off-diagonal elements) = **covariance of errors** between state variables i and j (how errors in one variable influence another).

Background Error Covariance=the uncertainty in the model forecast (background state) before assimilating new observations (Used in 3D-Var, 4D-Var, Kalman Filters, and EnKF)
Observation Error Covariance=uncertainty in the observations (e.g., satellite,)
Analysis Error Covariance=uncertainty in the analysis (final estimate after assimilation).
Model Error Covariance=uncertainties in the model dynamics (used in Kalman Filters to update state estimates)

Data Assimilation:

: Optimal Interpolation (OI) and Ensemble Adjustment Kalman Filter (EnAKF)

OI: the background error covariance matrix is stationary

❑It is a static, variance-minimizing method that updates the state estimate using a weighted average of observations and model forecasts.

❑The weights are determined based on a predefined covariance matrix, which does not evolve dynamically.

❑OI assumes stationary error statistics, meaning it does not adapt to time-varying uncertainties in the system.

Computationally efficient since it uses a precomputed covariance matrix.

Often used in operational weather forecasting where computational efficiency is key.

EnAKF: the background error covariance evolves with the model dynamics

❑It is an ensemble-based, sequential assimilation method that updates model states using a dynamically evolving estimate of error covariances.

❑Unlike OI, it does not require an explicit model for error covariances; instead, it estimates them from the ensemble of model states.

❑EAKF accounts for nonlinear and time-dependent error growth, making it more suitable for highly dynamic systems.

More computationally expensive because it requires running and updating an ensemble of forecasts.

Widely used in modern atmospheric and ocean data assimilation systems (e.g., for climate reanalysis and numerical weather prediction) due to its ability to handle complex error structures.

MINNI simulation setup over Europe: August 2023

resolution	0.15 x 0.1 lat/lon
number grid points	468x421
number of vertical levels	17
top of domain	11790m
meteorological driver	12 UTC IFS, 1 hrly
boundary conditions	CAMS global
Emission inventory	EmissionInventories6.1.1_year2022(operational end of 2024)

OI setup

'he most basic mathematical formulation of **Optimal Interpolation (OI)** for **satellite data assimilation** is
jiven by the **analysis equation**:

$$x^a = x^b + K(y - Hx^b)$$

vhere:

- x^a = **analysis state** (updated estimate of the atmosphere after assimilatio
- x^b = **background state** (forecast or prior estimate).
- y = **observation** (e.g., satellite temperature retrieval).
- H = **observation operator**, which converts the model state to observatio
- K = **Kalman gain matrix**, which determines how much weight is given to observations versus the background.
- $y - Hx^b$ = **observation innovation**, which represents the difference between the observed and predicted values.

Kalman Gain in OI

The **Kalman gain matrix** in OI is computed as:

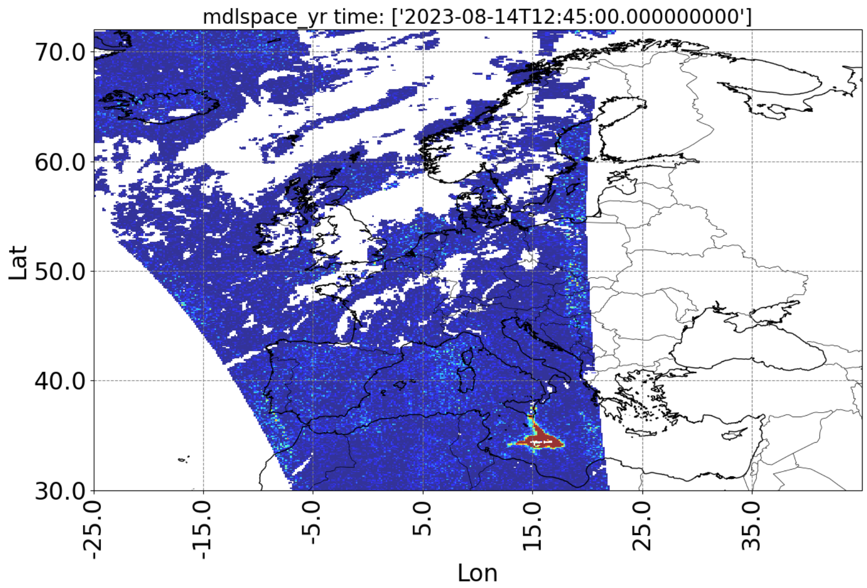
$$K = BH^T(HBH^T + R)^{-1}$$

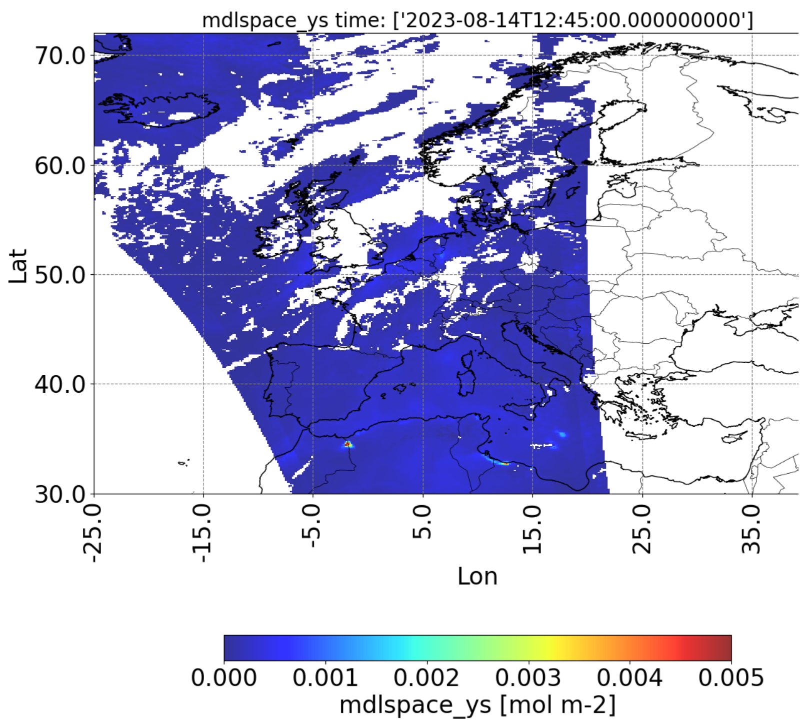
where:

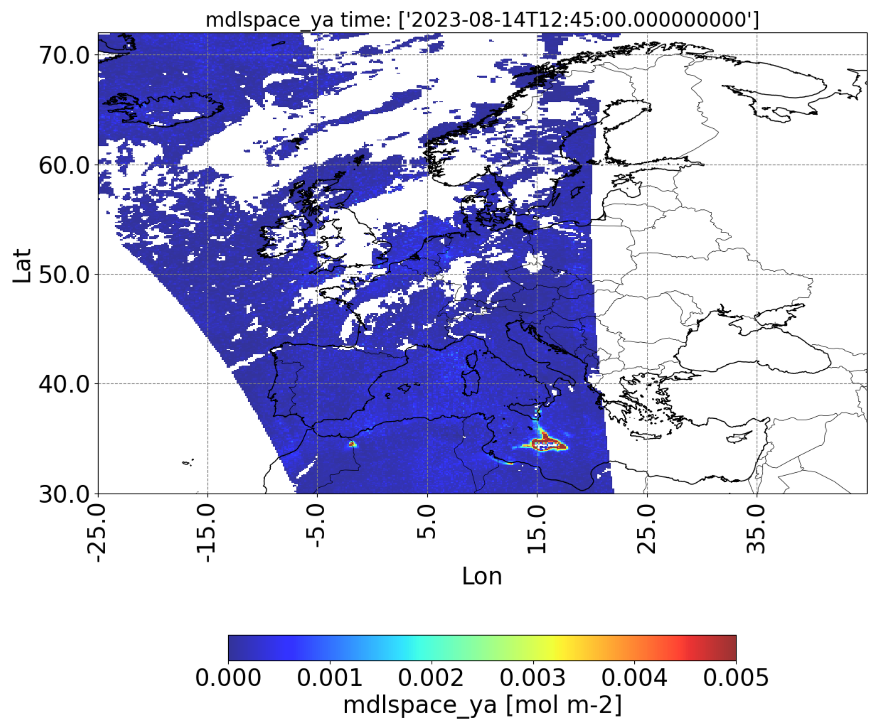
- B = **background error covariance matrix** (describes uncertainty in the background state).
- R = **observation error covariance matrix** (describes uncertainty in satellite observations).
- H^T = **transpose of the observation operator**, which transforms observation space back into model space.

Optimal Interpolation
Background Error Covariance Matrix (B) computed with NMC (Parrish and Derber, 1992) for 48h-0h forecast (D0 and D-2) using log concentration
B annual (average of monthly B), static
Negative values are not considered
Satellite data assimilated only if they are two times higher than their St.Dev
Observational Error Covariance Matrix (R) extracted from satellite data
B and R are diagonal: variance and correlation scales are handled separately

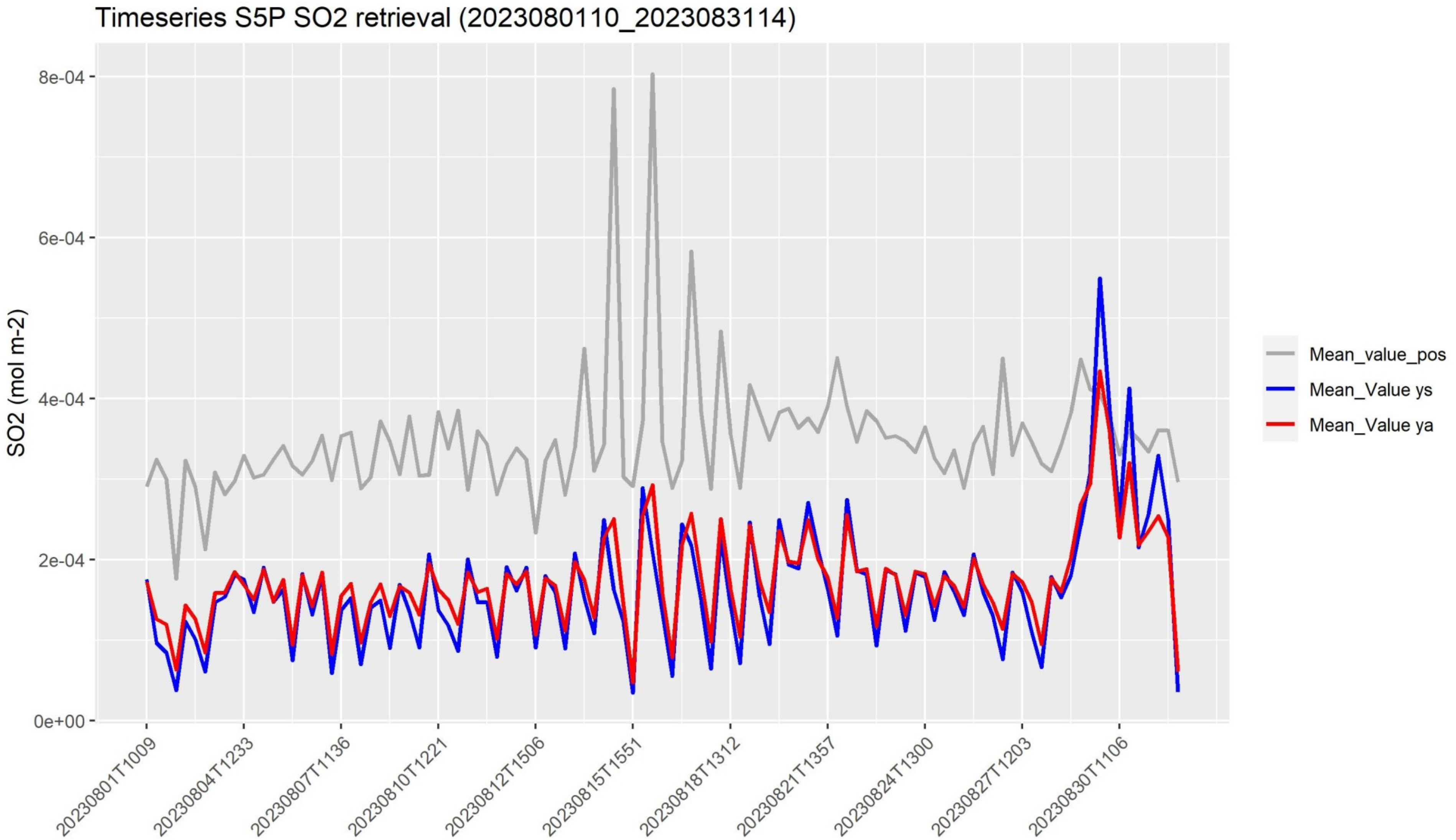
SO2 COBRA dataset assimilation with OI



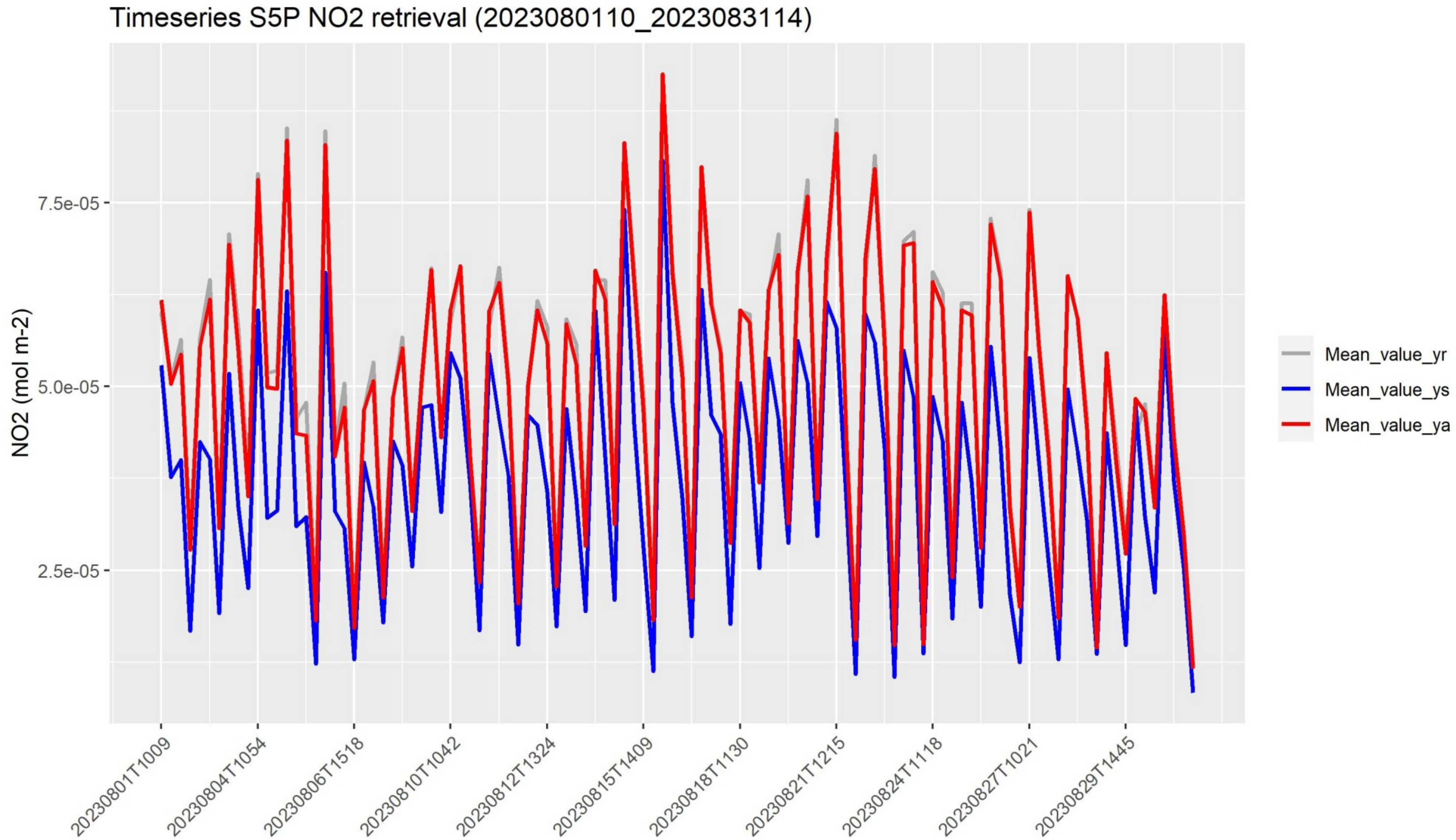




SO2 COBRA dataset assimilation with OI

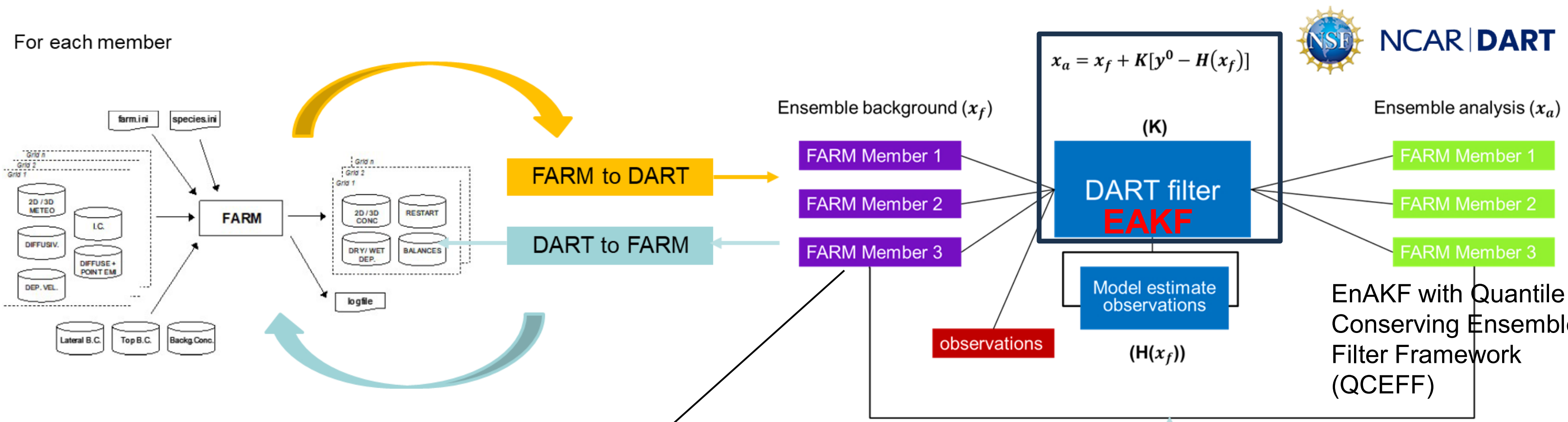


NO_2 dataset assimilation with OI



DART implementation in MINNI

Ensemble Adjustment Kalman Filter (EnAKF)



Perturbation FARM field consisting of varying emissions and BCs

FARM

ORCHESTRATOR

DART

Input.nml
- controls behavior
DART executables

FARM-DART

Sat Observation in DART format

https://dart.ucar.edu/

Sentinel 5P processed with Copernicus Satellite Operator
CSO
SO_2, HCHO, CO, O_3

ARIANET team: Alessandro D'Ausilio, Giorgia De Moliner and Camillo Silibello

A suez company

Emissions' perturbation for EAKF

Vertical correlation

$$A_{i,j,k,l=}\begin{cases} 1, \\ 0, \\ \dfrac{vcov}{\sqrt{1-a(i,j,k,l-1)^2}} \\ 0 \\ \dfrac{vcov}{\dfrac{vcov-\sum_{ll-1}A(i,j,l,ll)A(i,}{A(i,j,l,l)}} \\ \sqrt{1-a(i,j,k,l-1)^2} \end{cases}$$

k=1, l=1
k=1, l > 1
k=2, l = 1
k=2, l=2
k=2, l> 2
k>=3, l>1
k>=3, l < k
k>=3 l=ka

Horizontal correlation

$$w_{(i,j,k)} = exp(-(d_{ij}^2)/(L_{hz}^2\ ))$$

Box-Muller random field $$Z_{i,j,k} = B_{i,J,k}\sqrt{-2\ln(U_1)\cos(2\pi U_2)}$$

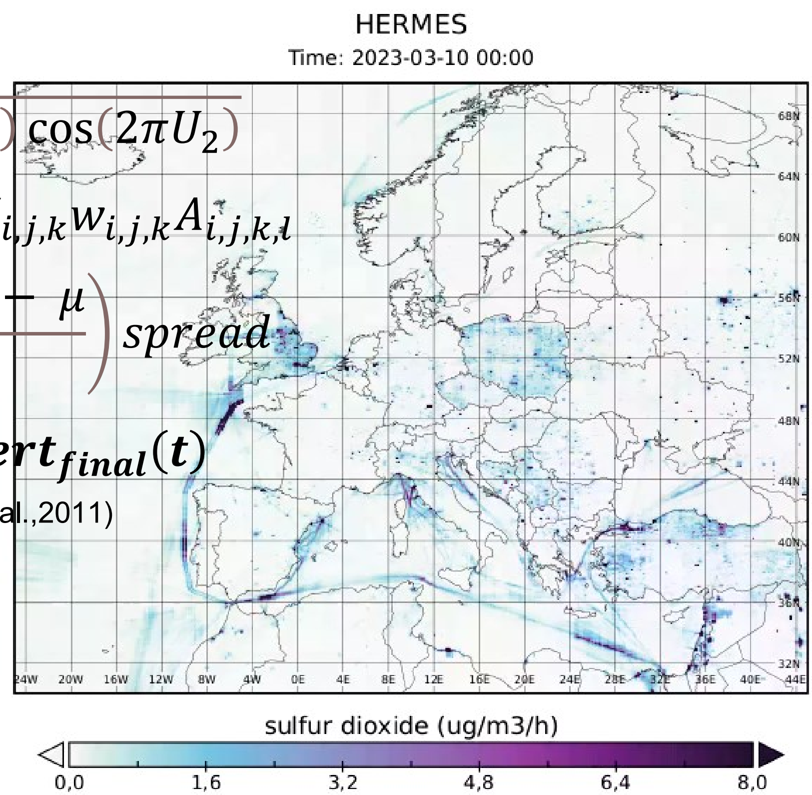
Applying horizontal and vertical corr. $$Pert_{i,j,k} = Z_{i,j,k}w_{i,j,k}A_{i,j,k,l}$$

Recentering and rescaling $$Pert_{final} = \left(\frac{Field-\mu}{\sigma}\right)spread$$

$$\boldsymbol{Pert_{final}(t) = \alpha Pert_{final}(t-1) + \sqrt{1-\alpha^2}Pert_{final}(t)}$$

(Boynard et al.,2011)

Time decorrelation $$\alpha = exp\left(-\frac{1}{\tau}\right)$$



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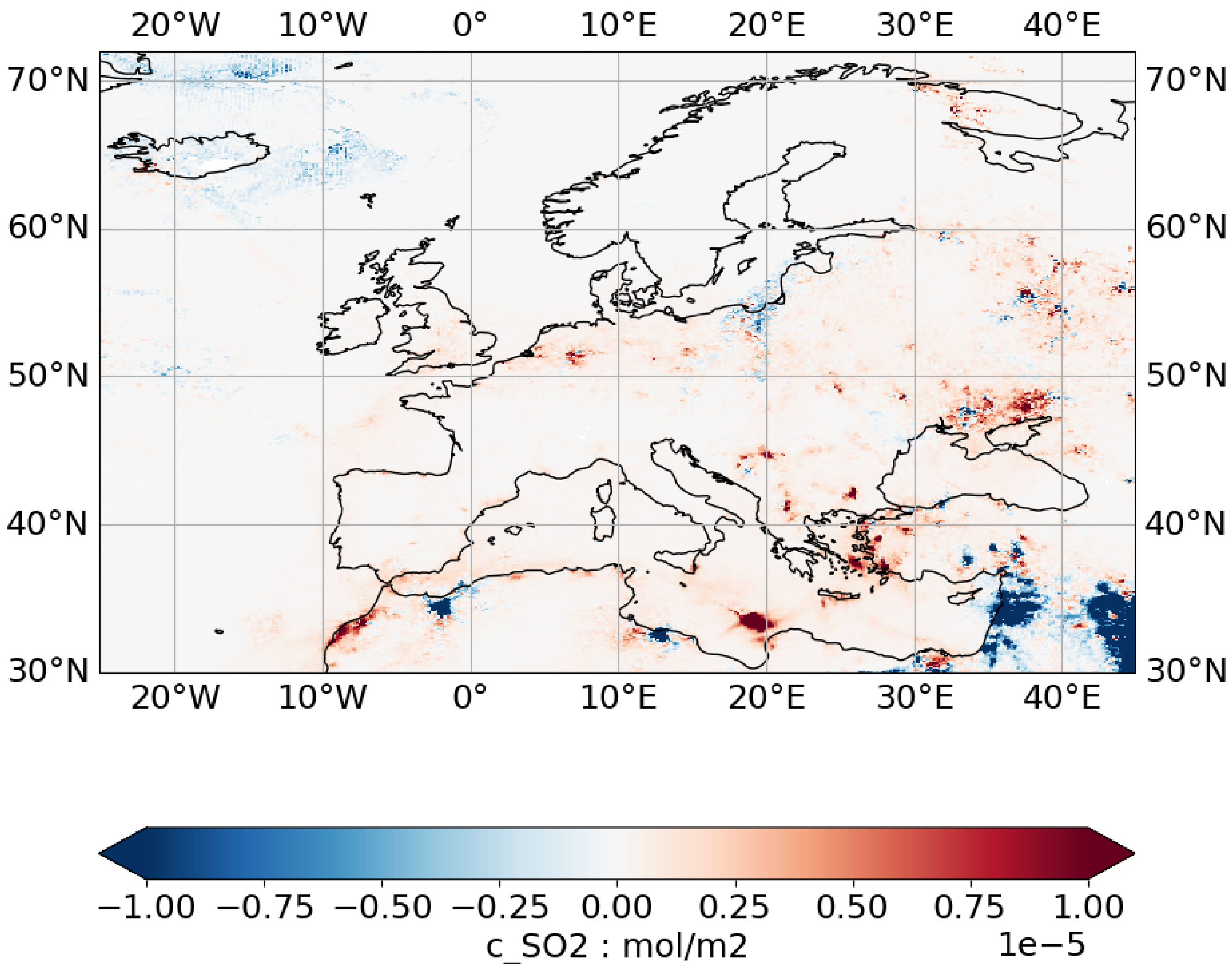
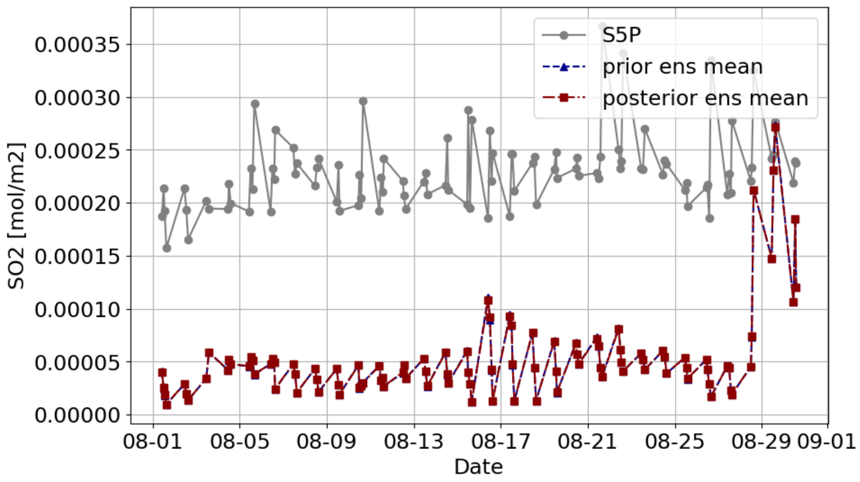
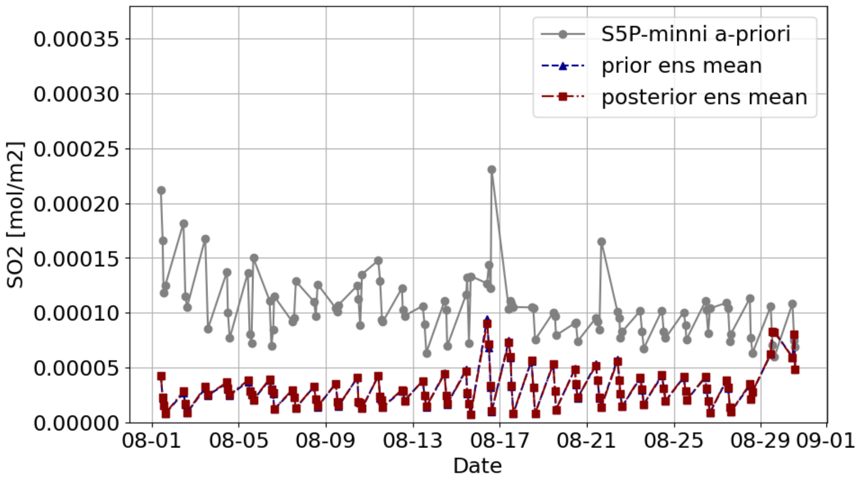
SO2 COBRA dataset assimilation with DART- EnAKF



Averaged difference between Posterior and Prior ensemble means

SO2 COBRA dataset assimilation with DART- EnAKF





Time-series of mean concentration averaged over the domain. Gray: retrieval. Blue: prior ensemble mean. Red: posterior ensemble mean. Left: a priori using the tm5 model. Right a priori using the MINNI model

Summary and future plans

-SO2 satellite data assimilation with OI makes “visible” Etna plume more than EAKF-DART with current setup

-HCHO, CO and O3 satellite data will be assimilated with OI and at least one pollutant with EAKF-DART

-study the sensitivity of OI results to background error covariance matrix specification

-study the sensitivity of SO2 results with EAKF-DART to perturbation parameters

-study if DART performances improves when SO2 Etna emissions will be included

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EGU 2025

EGU General Assembly 2025

EDI

Atmospheric Composition and Numerical Weather Forecasting

Co-sponsored by WMO and CAMS

Convener: Johannes Flemming

Co-conveners: Alexander Baklanov, Georg Grell, Sara Basart

- Orals | Tue, 29 Apr, 10:45–12:25 (CEST) Room M1
- Posters on site | Attendance Tue, 29 Apr, 14:00–15:45 (CEST) | Display Tue, 29 Apr, 14:00–18:00 Hall X5
- Posters virtual | Attendance Wed, 30 Apr, 14:00–15:45 (CEST) | Display Wed, 30 Apr, 14:00–18:00 vPoster spot 5

Session description

Orals: Tue, 29 Apr | Room M1

> The oral presentations are given in a hybrid format supported by a Zoom meeting featuring on-site and virtual presentations. The button to access the Zoom meeting appears just before the time block starts.

Chairpersons: Johannes Flemming, Sara Basart, Alexander Baklanov

12:15–12:25 | EGU25-16042 | ECS | On-site presentation

Assessing the impacts of assimilating SO2 TROPOMI retrievals with MINNI and DART at the European scale: a case study of the Mount Etna eruption

Alessandro D'Ausilio, Giorgia De Moliner, Camillo Silibello, Andrea Bolignano, Gino Briganti, Felicita Russo, and **Mihaela Mircea**

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EGU 2025

EDI

Satellite observations of tropospheric composition and pollution, analyses with models and applications

Convener: Andreas Richter

Co-conveners: Shima Bahramvash Shams, Cathy Clerbaux, Pieternel Levelt

- Orals | Mon, 28 Apr, 14:00–18:00 (CEST) Room 0.11/12
- Posters on site | Attendance Mon, 28 Apr, 10:45–12:30 (CEST) | Display Mon, 28 Apr, 08:30–12:30 Hall X5
- Posters virtual | Attendance Wed, 30 Apr, 14:00–15:45 (CEST) | Display Wed, 30 Apr, 14:00–18:00 vPoster spot 5

Session description

Orals: Mon, 28 Apr | Room 0.11/12

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Chairpersons: Andreas Richter, Shima Bahramvash Shams

Posters on site: Mon, 28 Apr, 10:45–12:30 | Hall X5

> The posters scheduled for on-site presentation are only visible in the poster hall in Vienna. If authors uploaded their presentation files, these files are linked from the abstracts below.

> **Display time:** Mon, 28 Apr, 08:30–12:30

X5.19 | EGU25-16722

Assimilation of SO2, CO, HCHO and O3 satellite data with Optimal Interpolation implemented in Atmospheric Modelling System MINNI

Andrea Bolignano, Mario Adani, Gino Briganti, Felicita Russo, and Mihaela Mircea