

# Correzione dei modelli fotochimici tramite osservazioni satellitari: dall'assimilazione dati all'inversione

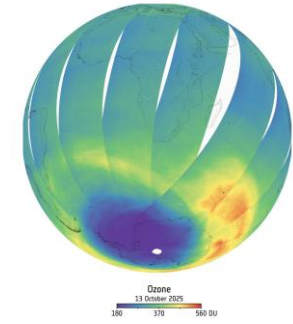
Giorgia De Moliner – PhD student



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2. Progetto europeo CAMEO: assimilazione in MINNI di totali colonnari di SO<sub>2</sub> su agosto 2023 ([ENEA](#), [ARIANET](#))
3. Correzione emissioni di NO<sub>x</sub> da osservazioni di NO<sub>2</sub> troposferico ([LISA/INERIS/ARIANET/POLIMI](#))

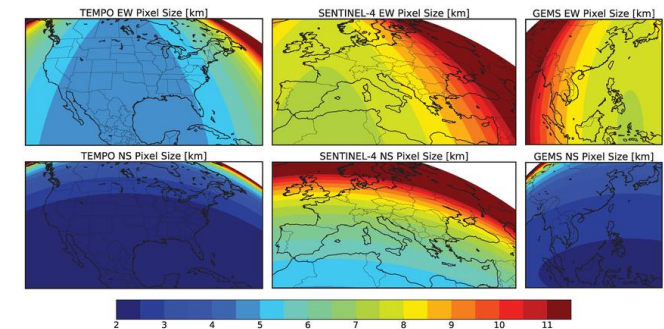
# Missioni europee per l'osservazione della composizione chimica dell'atmosfera



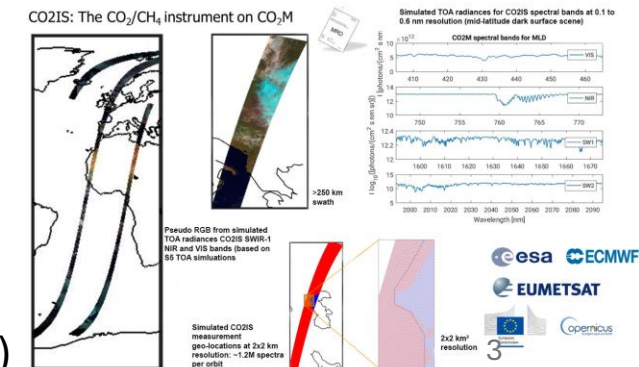
(S5P, S5)

Satellite	Instrument	Mission objectives	Resolution	Launch(operational) / EOL	Orbit	Provider	Links
Sentinel-5P	TROPOMI (UV-VIS-NIR-SWIR)	O3, CO, HCHO, NO2, SO2, CH4, Total Aerosols and Clouds	3.5x5km	2017(2018) to ≥2027	LEO, sun-synchronous, 1 day revisit time	ESA, NSO	<a href="https://space.oscar.wmo.int/instruments/view/tropomi">https://space.oscar.wmo.int/instruments/view/tropomi</a> <a href="https://sentiwiki.copernicus.eu/web/s5p-mission">https://sentiwiki.copernicus.eu/web/s5p-mission</a> <a href="https://stcorp.github.io/harp/doc/html/ingestions/index.html#sentinel-5p-products">https://stcorp.github.io/harp/doc/html/ingestions/index.html#sentinel-5p-products</a>
MetOp-SG-A1	Sentinel-5(A) (UV-VIS-NIR-SWIR), (+IASI-NG)	O3, CO, CO2, H2O, HCHO, NO2, SO2, CH4, OCHCHO, BrO	7km	2025(?) to 2034	LEO, sun-synchronous, 1 day revisit time	EUMETSAT, ESA	<a href="https://user.eumetsat.int/resources/user-guides/metop-sg-sentinel-5-uvns-11b-data-guide">https://user.eumetsat.int/resources/user-guides/metop-sg-sentinel-5-uvns-11b-data-guide</a> <a href="https://www.esa.int/Applications/Observing_the_Earth/Copernicus/Sentinel-5/Sentinel-5_debuts_images_of_atmospheric_gases">https://www.esa.int/Applications/Observing_the_Earth/Copernicus/Sentinel-5/Sentinel-5_debuts_images_of_atmospheric_gases</a>
Meteosat Third Generation (MTG-S1)	Sentinel-4 (UV-VIS-NIR)	BrO, HCHO, NO2, O3, SO2 and aerosol; also cloud top height	8km	2025(?) to 2036	GEO, European area, 1 hour revisit time	ESA, EUMETSAT	<a href="https://space.oscar.wmo.int/instruments/view/sentinel4">https://space.oscar.wmo.int/instruments/view/sentinel4</a> <a href="https://www.eumetsat.int/first-copernicus-sentinel-4-images-showcase-europes-hourly-air-pollution-watch">https://www.eumetsat.int/first-copernicus-sentinel-4-images-showcase-europes-hourly-air-pollution-watch</a>
CO2M-A, CO2M-B and CO2M-C	CO2I/CLIM/MAP (VIS/NIR/SWIR)	CO2, CH4 and NO2 (emissions)	0.8 km	2027/8/9 to 2034/5/6	LEO, sun-synchronous, 2- 3/5 days revisit time	ESA	<a href="#">Tracking human emissions from space</a> <a href="https://www.eoportal.org/satellite-missions/co2m#missionstatus">https://www.eoportal.org/satellite-missions/co2m#missionstatus</a>

(S4)



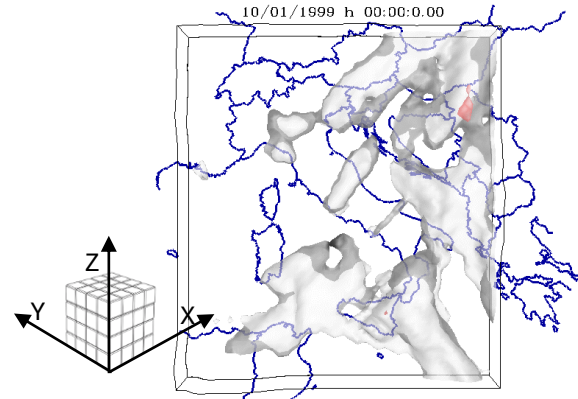
Castellanos, P.; Da Silva, A.M.; Darmenov, A.S.; Buchard, V.; Govindaraju, R.C.; Ciren, P.; Kondragunta, S. A Geostationary Instrument Simulator for Aerosol Observing System Simulation Experiments. *Atmosphere* **2019**, *10*, 2. <https://doi.org/10.3390/atmos10010002>



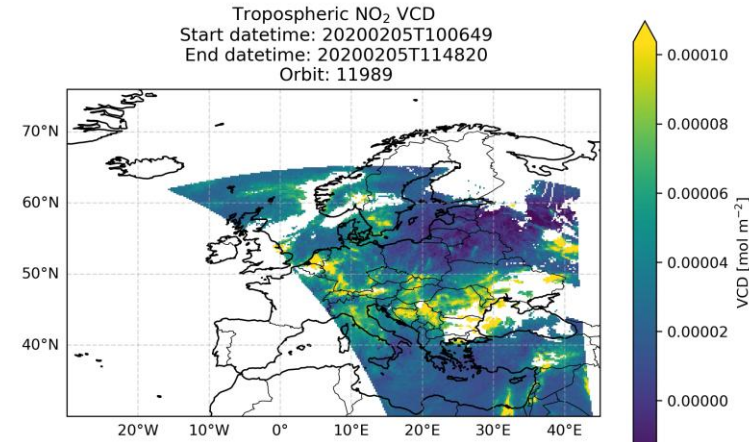
(CO2M)

<https://www.eumetsat.int/CO2M-TOA-TDS>

# Assimilazione Dati



Simulazioni



Osservazioni

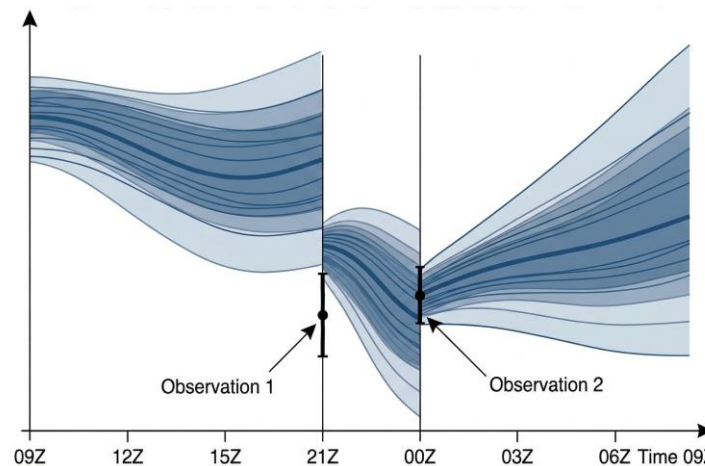
## Ensemble Kalman Filter

$P$

$$\begin{bmatrix} \sigma_{00}^2 & \sigma_{01}^2 & \sigma_{02}^2 \\ \sigma_{10}^2 & \sigma_{11}^2 & \sigma_{12}^2 \\ \sigma_{20}^2 & \sigma_{21}^2 & \sigma_{22}^2 \end{bmatrix}$$



$\{0, \dots, N\}$



$$\begin{aligned} \mathbf{x}^a(t) &= \mathbf{x}^f(t) + \mathbf{K}[\mathbf{y}^o - \mathcal{H}\mathbf{x}^f(t)], \\ \mathbf{K} &= \mathbf{P}^f \mathcal{H}^T (\mathcal{H} \mathbf{P}^f \mathcal{H}^T + \mathbf{R})^{-1}, \\ \mathbf{x}^f(t+1) &= \mathcal{M}[\mathbf{x}^a(t)]. \end{aligned}$$

# Il progetto CAMEO



Funded by the European Union

COORDINATED BY  
**ECMWF**



Atmosphere  
Monitoring



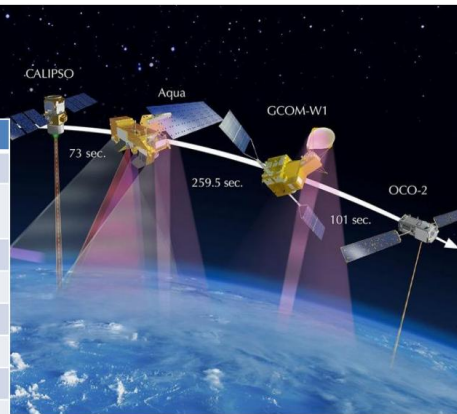
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## AC observations used in CAMS global

Species	Instruments
CAMS NRT	
O <sub>3</sub>	<b>S5P, GOME-2, OMI, OMPS-NP, MLS, OMPS-LP, GEMS</b>
CO	<b>S5P, IASI, MOPITT</b>
NO <sub>2</sub>	<b>S5P, GOME-2, GEMS</b>
Aerosol	<b>MODIS, VIIRS, PMAp, S3</b>
CO <sub>2</sub>	<b>GOSAT, IASI, OCO-2</b>
CH <sub>4</sub>	<b>GOSAT, IASI, S5P</b>
SO <sub>2</sub> (volcanic)	<b>S5P, GOME-2, IASI</b>
SO <sub>2</sub> (anthropogenic)	<b>S5P</b>
HCHO	<b>S5P</b>
GFAS fire emissions	<b>MODIS, VIIRS, GOES, S3</b>



CAMS uses Earth Observation data from many satellites for atmospheric composition and weather.

---- Used  
---- Undergoing testing



Melanie Ades (ECMWF)  
[https://events.ecmwf.int/event/498/contributions/5446/attachments/3507/5919/DA\\_training\\_Course\\_AC\\_March\\_2026\\_Ades.pdf](https://events.ecmwf.int/event/498/contributions/5446/attachments/3507/5919/DA_training_Course_AC_March_2026_Ades.pdf)

4

- Core of MINNI, operationally run to get **CAMS European air quality forecasts** in a multi-model approach



11-member  
ensemble  
10km Europe

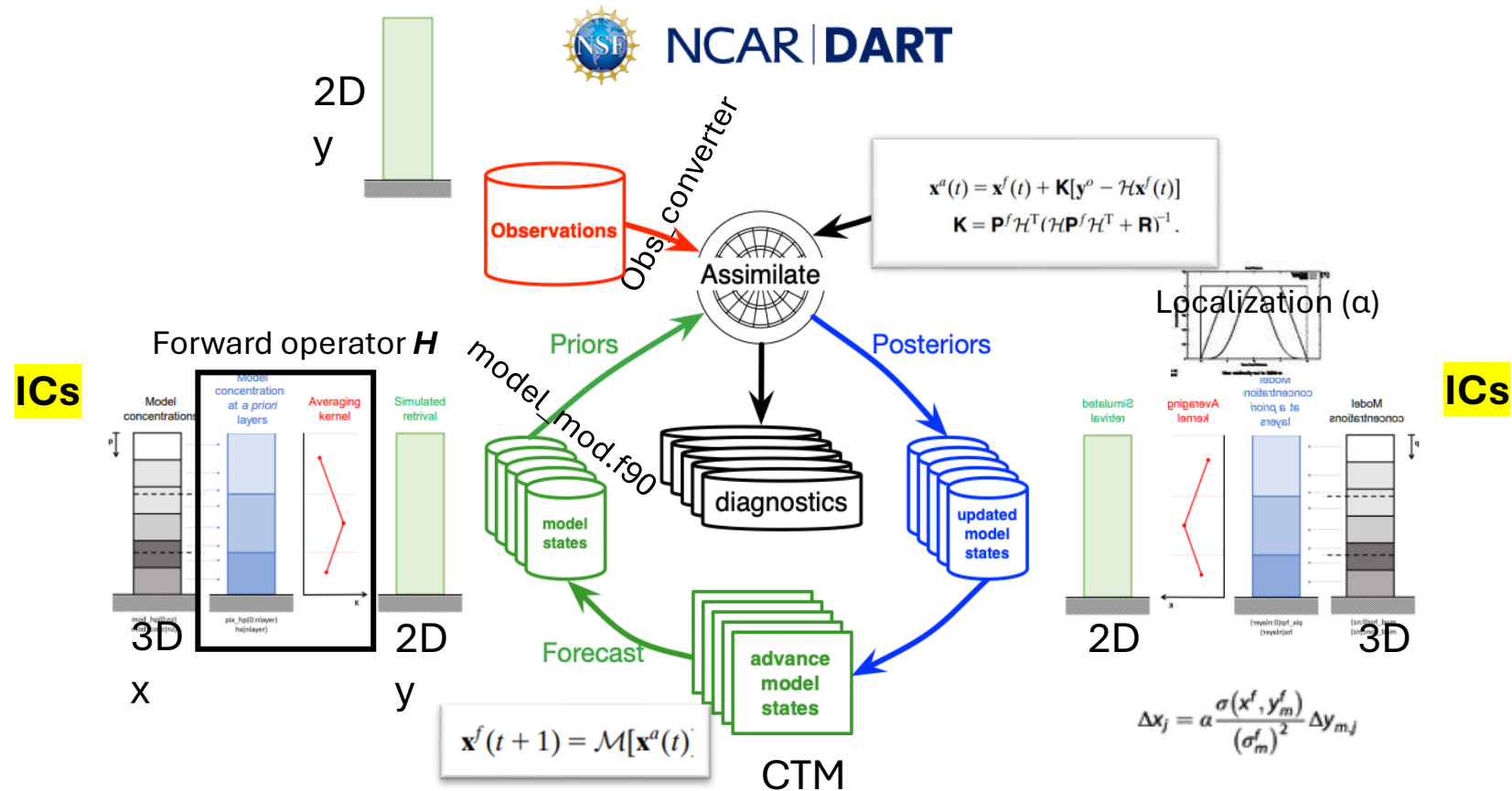


<https://atmosphere.copernicus.eu/european-air-quality-forecast-plots>

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"The CAMEO project (grant agreement No101082125) is funded by the European Union. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Commission. Neither the European Union nor the granting authority can be held responsible for them."

# DART workflow



[1] J. L. Anderson, "A local least squares framework for ensemble filtering," *Monthly Weather Review*, vol. 131, no. 4, 2003, doi: 10.1175/1520-0493(2003)131<0634:ALLSFF>2.0.CO;2.



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<https://doi.org/10.5194/egusphere-egu25-16042>

EGU General Assembly 2025

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# Assessing the impacts of assimilating SO<sub>2</sub> TROPOMI retrievals with MINNI and DART at the European scale: a case study of the Mount Etna eruption

Alessandro D'Ausilio<sup>1</sup>, Giorgia De Moliner<sup>2</sup>, Camillo Silibello<sup>1</sup>, Andrea Bolignano<sup>3</sup>, Gino Briganti<sup>3</sup>, Felicità Russo<sup>3</sup>, and Mihaela Mircea<sup>3</sup>

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<sup>2</sup>Department of Civil and Environmental Engineering, Politecnico di Milano, Piazza Leonardo da Vinci 32, Milan, 20133, Italy (giorgia.demoliner@polimi.it)

<sup>3</sup>Italian National Agency for New Technologies, Energy and Sustainable Economic Development (ENEA), Via Martiri di Monte Sole 4, 40129 Bologna, Italy (mihaela.mircea@enea.it)

Article

# Assimilation of SO<sub>2</sub> TROPOMI retrievals at the European scale with EnAKF implemented in MINNI through DART

Giorgia De Moliner<sup>2</sup>, Alessandro D'Ausilio<sup>1</sup>, Andrea Bolignano<sup>3</sup>, Gino Briganti<sup>3</sup>, Felicita Russo<sup>3</sup>, Massimo D'Isidoro<sup>3</sup>,  
Giovanni Lonati<sup>2</sup>, Mihaela Mircea<sup>3</sup>

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- <sup>2</sup> Department of Civil and Environmental Engineering, Politecnico di Milano, Piazza Leonardo da Vinci 32, Milan, 20133, Italy 10-11
- <sup>3</sup> Models and Measures for Air Quality and Climate Observation Laboratory, Italian National Agency for New Technologies, Energy and Sustainable Economic Development – ENEA, Bologna, 40121 12-13
- \* Correspondence: 14
- † These authors contributed equally to this work. 15

**Abstract:** XXXXXXXX 16

**Keywords:** Sulphur Dioxide, Data Assimilation, Ensemble Kalman Filter, Sentinel-5P, TROPOMI, air quality modelling 17-18

(Draft) 19

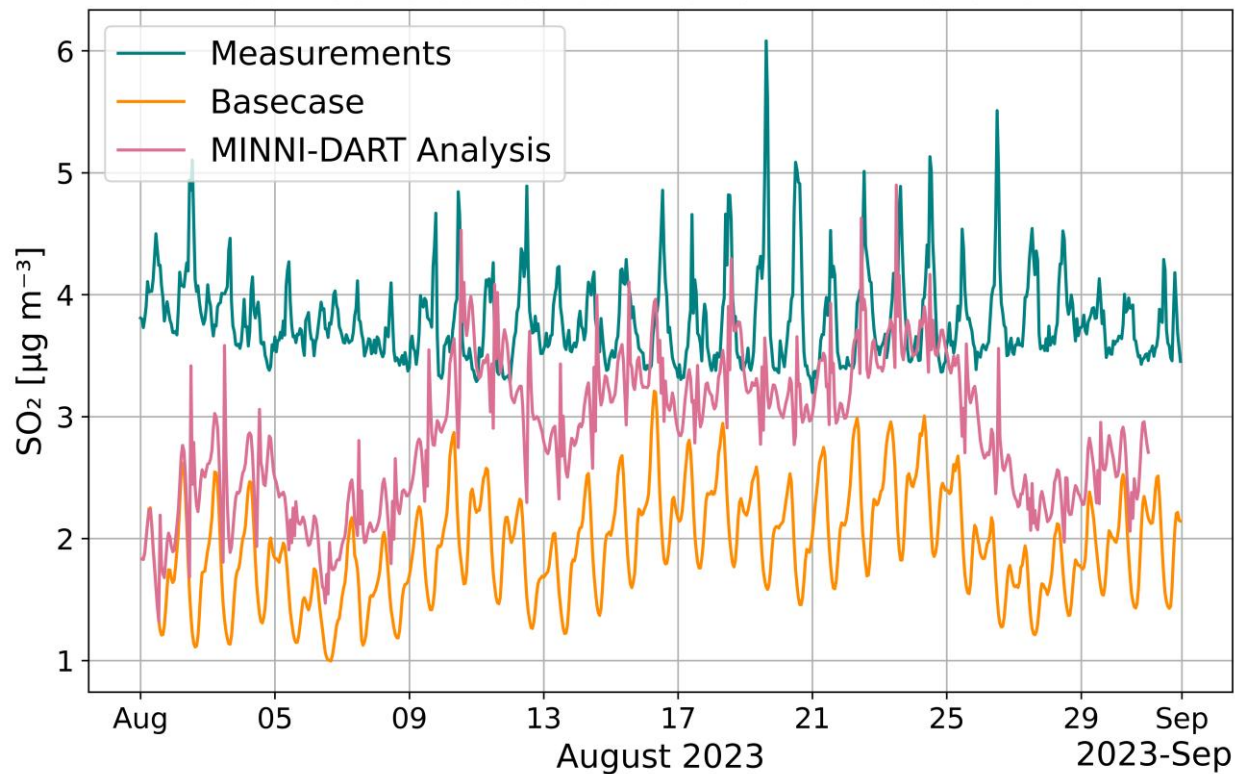


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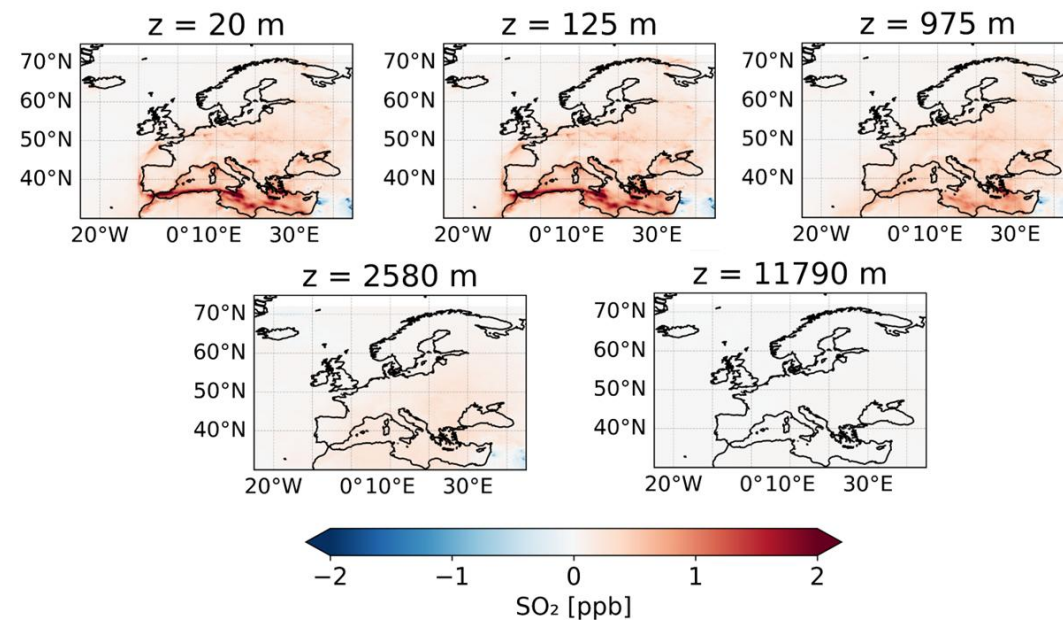


# Lo spazio del modello (3D)

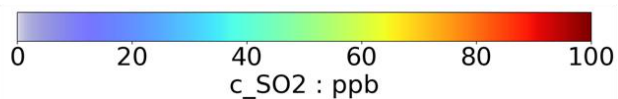
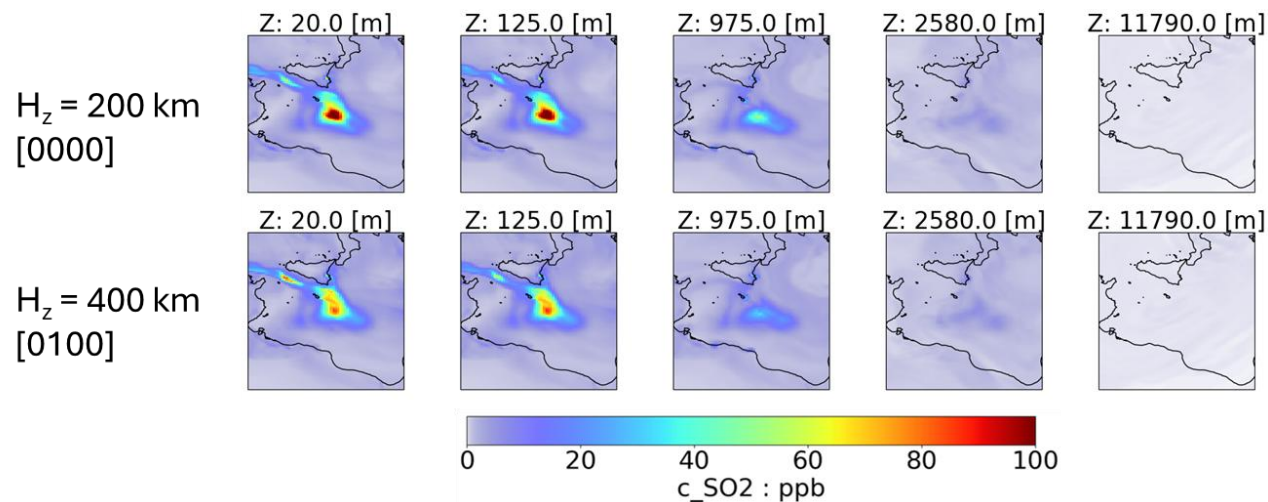
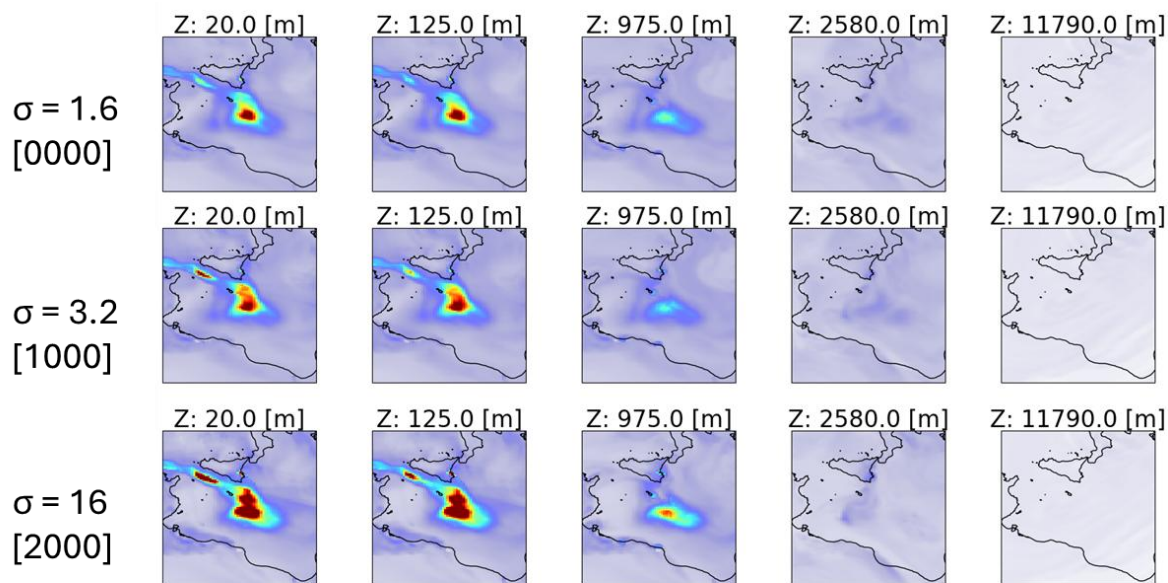
SO<sub>2</sub> Surface Concentration - EEA Stations



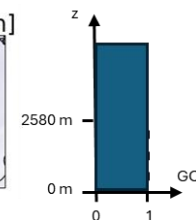
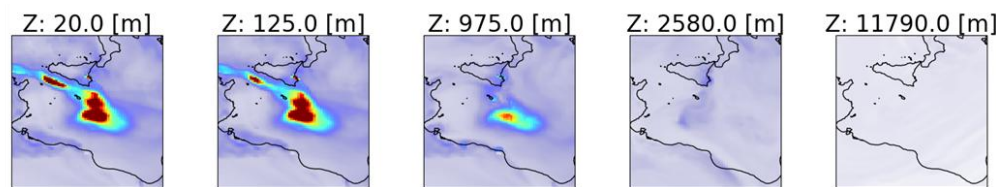
Monthly Mean Total Column SO<sub>2</sub> Difference (Analysis - Basecase)



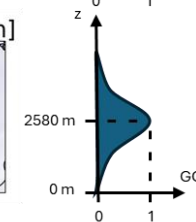
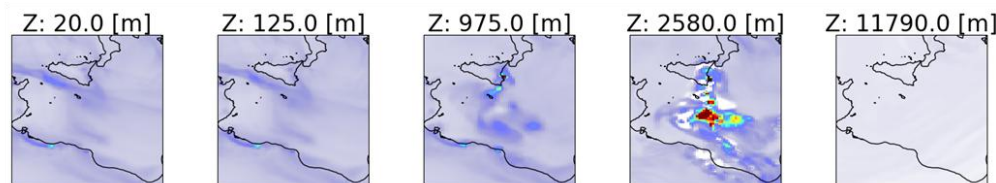
# Analisi di sensibilità



No vertical localization [2000]

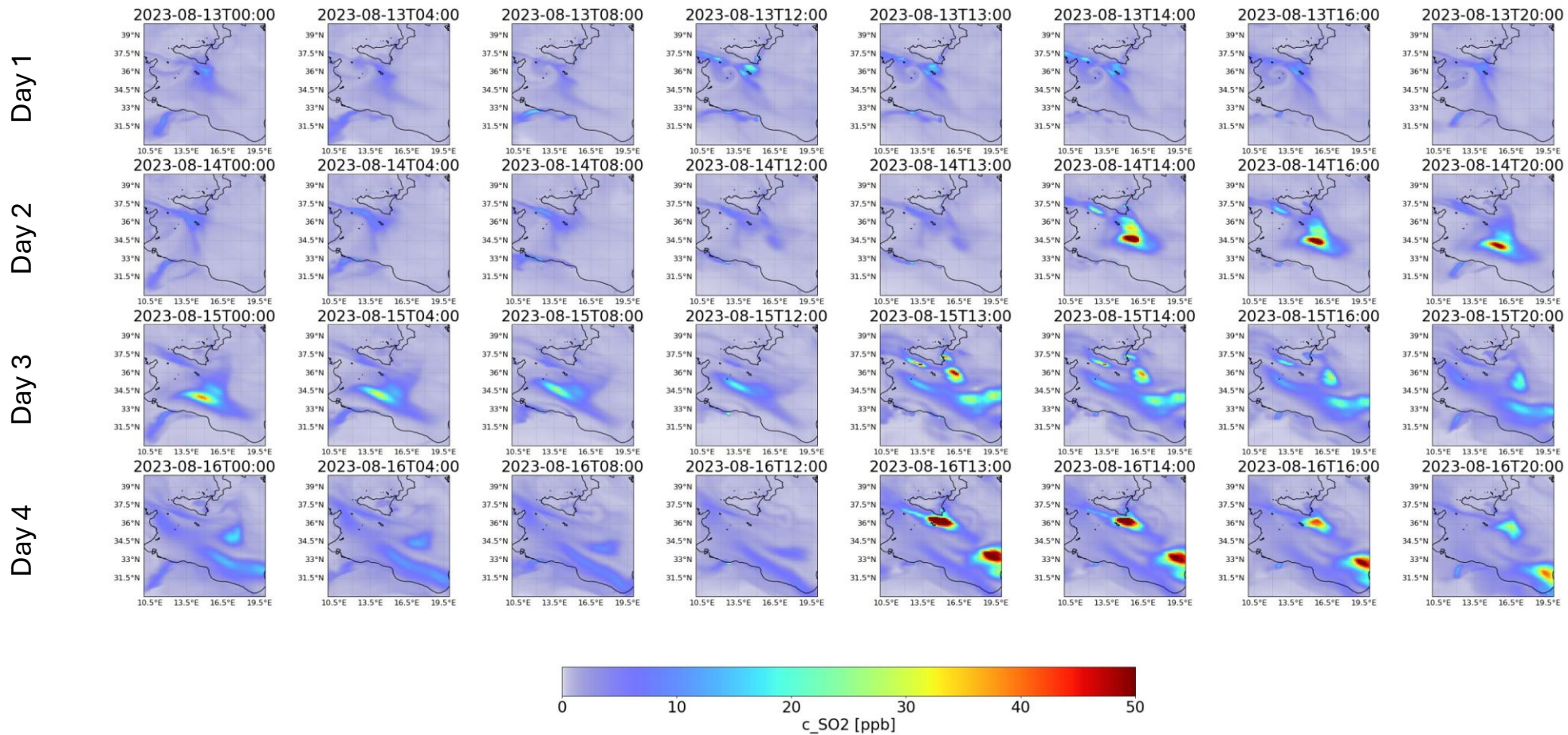


Vertical localization (GC) [2010]



# Persistenza della correzione

SO<sub>2</sub> Concentrations over time at z=20m



# Inverse Modeling

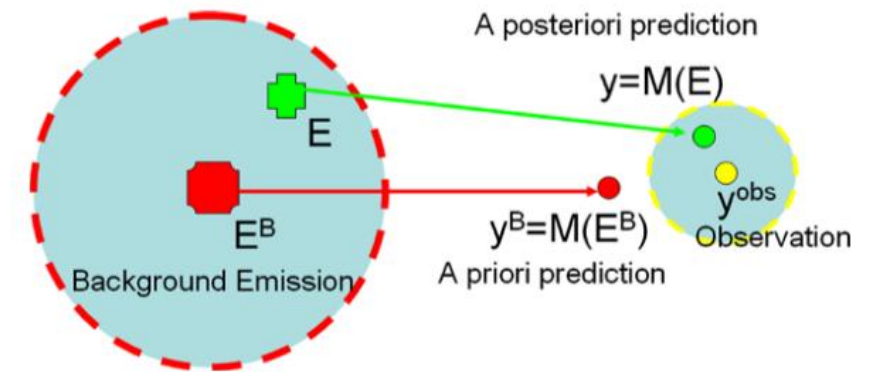
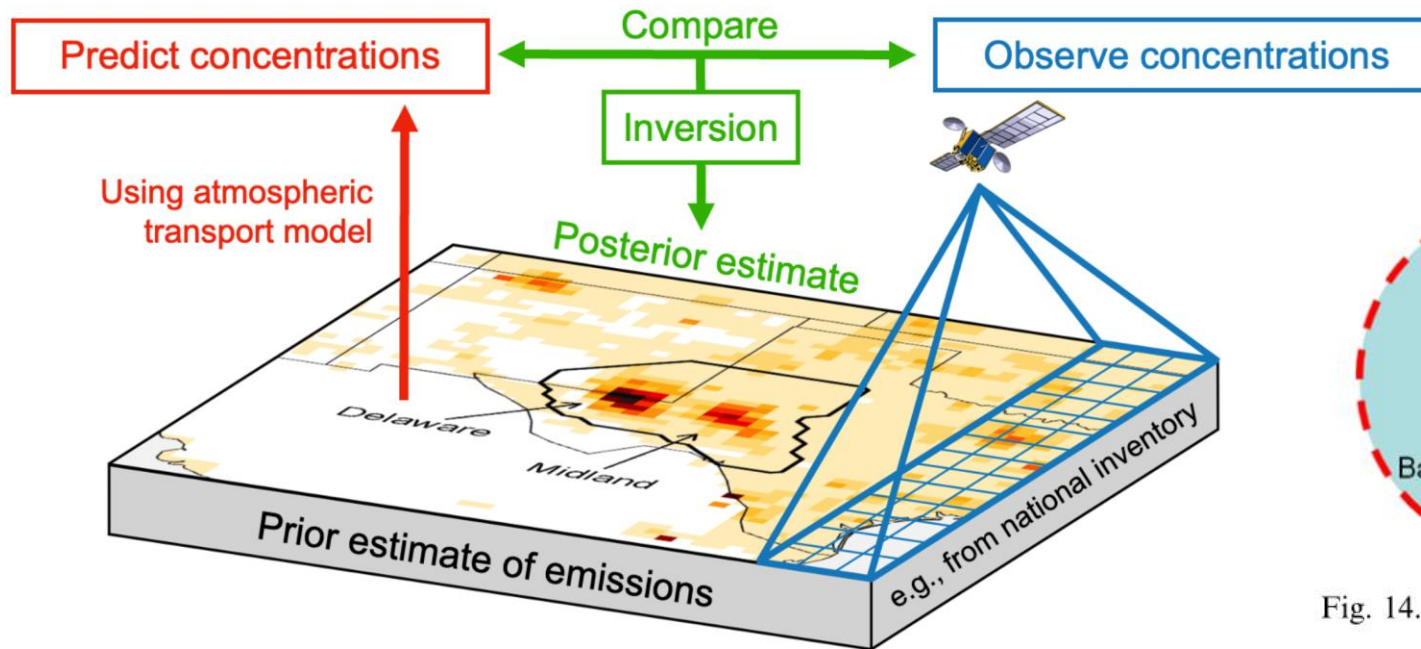


Fig. 14. A-basic methodology of top-down estimates of emissions.

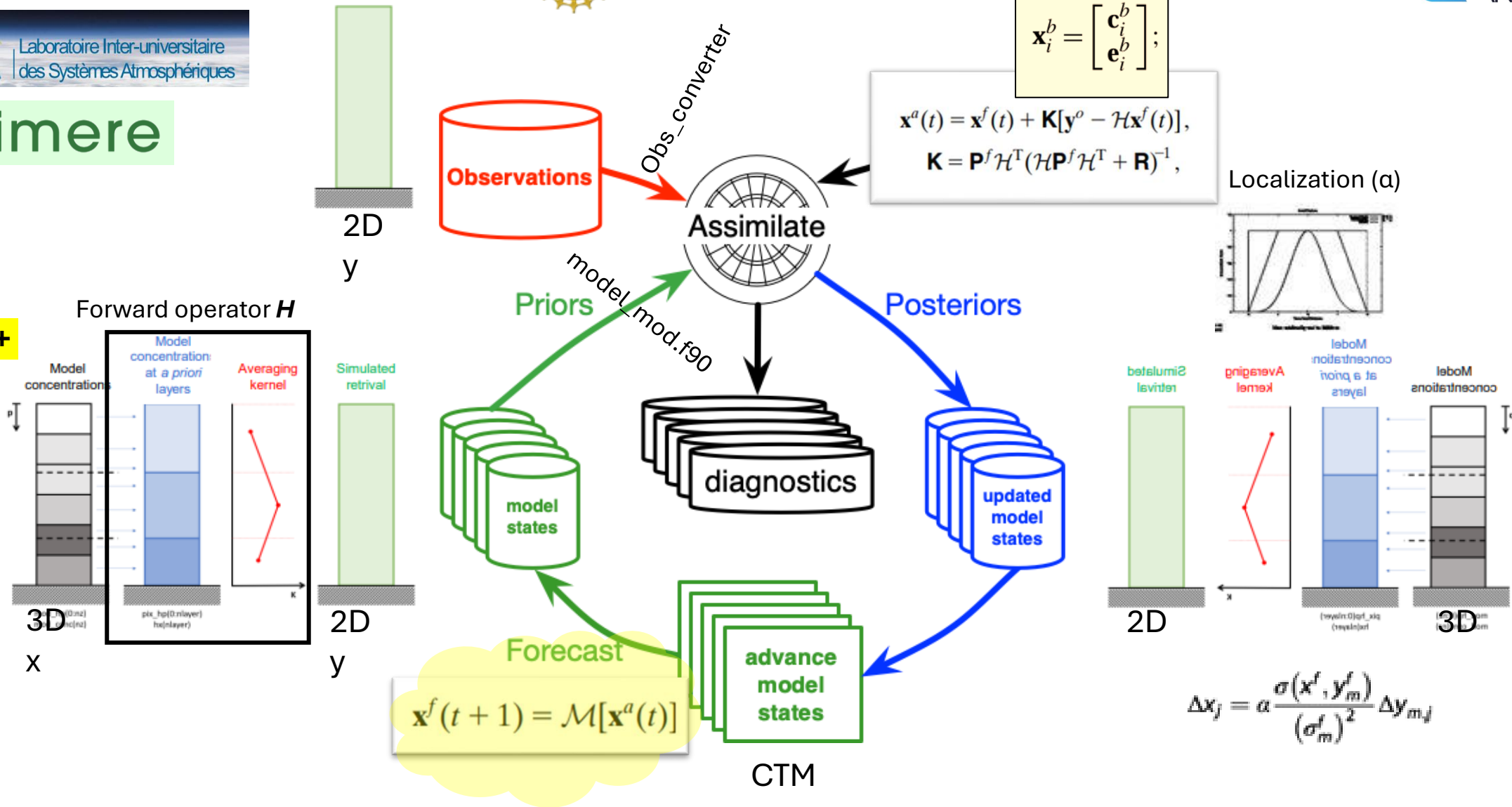
<https://carboninversion.com/about/>

Varon, D. J., Jacob, D. J., Sulprizio, M., Estrada, L. A., Downs, W. B., Shen, L., Hancock, S. E., Nesser, H., Qu, Z., Penn, E., Chen, Z., Lu, X., Lorente, A., Tewari, A., and Randles, C. A.: Integrated Methane Inversion (IMI 1.0): a user-friendly, cloud-based facility for inferring high-resolution methane emissions from TROPOMI satellite observations, *Geosci. Model Dev.*, 15, 5787–5805, <https://doi.org/10.5194/gmd-15-5787-2022>, 2022.

Gregory R. Carmichael, et al. 2008 ,  
<https://doi.org/10.1016/j.jcp.2007.02.024>.)

**EMI + ICs**

**EMI + ICs**

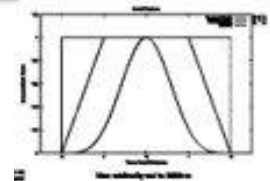


$$\mathbf{x}_i^b = \begin{bmatrix} \mathbf{c}_i^b \\ \mathbf{e}_i^b \end{bmatrix};$$

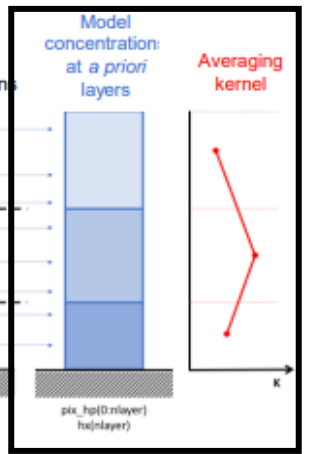
$$\mathbf{x}^a(t) = \mathbf{x}^f(t) + \mathbf{K}[\mathbf{y}^o - \mathcal{H}\mathbf{x}^f(t)],$$

$$\mathbf{K} = \mathbf{P}^f \mathcal{H}^T (\mathcal{H} \mathbf{P}^f \mathcal{H}^T + \mathbf{R})^{-1},$$

Localization ( $\alpha$ )



Forward operator  $\mathcal{H}$



$$\Delta x_j = \alpha \frac{\sigma(x'_j, y'_m)}{(\sigma'_m)^2} \Delta y_{m,j}$$

[1] J. L. Anderson, "A local least squares framework for ensemble filtering," *Monthly Weather Review*, vol. 131, no. 4, 2003, doi: 10.1175/1520-0493(2003)131<0634:ALLSFF>2.0.CO;2.

# EGU2026

EDI\*

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

Convener: Andreas Richter | Co-conveners: Cathy Clerbaux, Pieter Levelt, Miriam Latsch<sup>EC5</sup>

▶ Orals | Fri, 08 May, 08:30–12:30 (CEST), 14:00–15:45 (CEST) ■ Room E2

▶ Posters on site | Attendance Thu, 07 May, 14:00–15:45 (CEST) | Display Thu, 07 May, 14:00–18:00 ■ Hall X5



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<https://doi.org/10.5194/egusphere-egu26-12084>  
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Poster | Thursday, 07 May, 14:00–15:45 (CEST), Display time Thursday, 07 May, 14:00–18:00 ■ Hall X5, X5.13

## Refining NO<sub>x</sub> Emissions using Satellite Observations: Inverse Modeling through DART-CHIMERE Data Assimilation of S5P/TROPOMI NO<sub>2</sub> Retrievals

Giorgia De Moliner<sup>1</sup>, Gaëlle Dufour<sup>2</sup>, Gaël Descombes<sup>3</sup>, Alessandro D'Ausilio<sup>4</sup>, Adriana Coman<sup>2</sup>, Guillaume Siour<sup>5</sup>, Arineh Cholakian<sup>5</sup>, and Giovanni Lonati<sup>1</sup>

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<sup>2</sup>Université Paris Cité and Univ Paris Est Créteil, CNRS, LISA, Paris, 75013, France

<sup>3</sup>Institut National de l'Environnement Industriel et des Risques (INERIS), Parc Alata, BP2, 60550 Verneuil-en-Halatte, France

<sup>4</sup>Arianet srl, 20159 Milano, Via Benigno Crespi 52, Italy

<sup>5</sup>Laboratoire de Météorologie Dynamique (LMD)/IPSL, Ecole Polytechnique, Institut Polytechnique de Paris, ENS, Université PSL, Sorbonne Université, CNRS, Route de Saclay, Palaiseau, 91128, France

Emission inventories data used in chemical transport models (CTMs) are subject to uncertainties that propagate into air quality simulations. Air quality data from satellite observations can provide additional constraints on emissions, enabling a top-down approach that complements conventional bottom-up inventories.

In this work, we performed an inverse modeling within the framework of the DART-CHIMERE data assimilation system. A state vector augmentation method is applied to NO<sub>x</sub> emission fields, allowing emissions to be adjusted along with initial chemical concentrations. This approach aims to mitigate the limited persistence of corrections obtained through initial-condition-only assimilation, which are often damped by CTM dynamics.

The methodology is tested over the European domain for S5P/TROPOMI NO<sub>2</sub> total column retrievals, and the impact of emission adjustments is evaluated using independent surface NO<sub>2</sub> measurements from ground-based monitoring stations. First results based on a test case are presented to illustrate the potential of the approach. While the approach does not aim to replace established bottom-up inventories, the results indicate that satellite-informed emission corrections can provide additional, dynamically consistent constraints, supporting their use as a complementary component in CTM-based air quality analyses.

**How to cite:** De Moliner, G., Dufour, G., Descombes, G., D'Ausilio, A., Coman, A., Siour, G., Cholakian, A., and Lonati, G.: Refining NO<sub>x</sub> Emissions using Satellite Observations: Inverse Modeling through DART-CHIMERE Data Assimilation of S5P/TROPOMI NO<sub>2</sub> Retrievals, EGU General Assembly 2026, Vienna, Austria, 3–8 May 2026, EGU26-12084, <https://doi.org/10.5194/egusphere-egu26-12084>, 2026.

# Inverse Modeling – le tecniche

Methodology	Technique	Description & Technical Characteristics	Key References (Yaer, Species, Obs, CTM) with focus on satellite observations
1. Advanced Data Assimilation	Ensemble Methods (LETKF, EAKF)	Updates emissions by calculating covariance between ensemble states and observations. Allows for simultaneous state/parameter updates ( <b>Joint Estimation</b> ).	<ul style="list-style-type: none"> <li>Hsu et al. (2024; <b>NOx</b>, OSSE of TEMPO vs TROPOMI, <b>WRF-Chem/DART</b>);</li> <li>Liu et al. (2017; <b>NOx</b>, OSSE of TEMPO, <b>WRF-Chem/DART</b>);</li> <li>Miyazaki et al. (2012a,b, 2013, 2017; <b>NOx among others</b>, OMI/GOME-2/SCIAMACHY/MOPITT/MLS, <b>CHASER/MIROC-Chem/LETKF</b>, <a href="https://doi.org/doi:10.5194/acpd-11-31523-2011">https://doi.org/doi:10.5194/acpd-11-31523-2011</a>);</li> <li>Gaubert, B., et al. (2020; <b>CO</b>, MOPITT, <b>CAM-Chem/DART</b>, <a href="https://doi.org/10.5194/acp-20-14617-2020">https://doi.org/10.5194/acp-20-14617-2020</a>);</li> </ul>
	3/4D-Variational (3/4D-Var)	Minimizes a cost function over a time window using an adjoint model to find the optimal emission gradient backwards in time. Allows <b>Joint Estimation</b> .	<ul style="list-style-type: none"> <li>Elbern et al. (2007; <b>NOx</b>, Ground-based, <b>EUROAD</b>);</li> <li>Chai et al. (2009; <b>NOx</b>, SCIAMACHY, <b>STEM</b>);</li> <li>Botero et al. (2021; <b>NOx</b>, TROPOMI, <b>LOTOS-EUROS</b>);</li> <li>Savas et al. (2023; <b>NOx</b>, OMI, <b>CHIMERE</b>);</li> <li>Zhang et al. (2019; <b>CO and NOx</b>, MOPITT, OMI, TES, and OSIRIS, <b>GEOS-Chem</b>, <a href="https://doi.org/10.1029/2018JD028670">https://doi.org/10.1029/2018JD028670</a>);</li> </ul>
2. Mass Balance & Top-Down	Flux-Divergence / Plume Fitting	Uses the continuity equation to isolate emissions via <b>horizontal transport divergence and chemical loss</b> . Ideal for point sources.	<ul style="list-style-type: none"> <li>Beirle et al. (2021; <b>NOx</b>, TROPOMI, <b>Offline</b>);</li> <li>Chen et al. (2025; <b>SO2</b>, TROPOMI, <b>Offline</b>);</li> </ul>
	Scaling Factors / Mass Balance	Directly adjusts emissions based on the <b>ratio between observed and modeled columns</b> .	<ul style="list-style-type: none"> <li>Streets et al. (2013; <b>Review</b>, Various, Various);</li> <li>Mun et al. (2023; <b>Review</b>, <b>NOx</b>, OSSE, <a href="https://doi.org/10.1016/j.atmosenv.2022.119429">https://doi.org/10.1016/j.atmosenv.2022.119429</a>);</li> <li>Leue et al. (2001, <b>NOx</b>, GOME, <b>Mass Balance</b>, <a href="https://doi.org/10.1029/2000JD900572">https://doi.org/10.1029/2000JD900572</a>, <a href="#">pioneering study</a>);</li> </ul>
3. Hybrid	DECSO (Daily Inversion)	It calculates <b>sensitivity trajectories</b> to see how a change in emissions at a specific grid cell affects the satellite pixel downwind. It updates the emission inventory daily. Optimized for short-lived species on a regional scale. Allows <b>Joint Estimation</b> .	<ul style="list-style-type: none"> <li>Mijling &amp; van der A (2012; <b>NOx</b>, OMI/GOME-2, <b>CHIMERE</b>);</li> </ul>

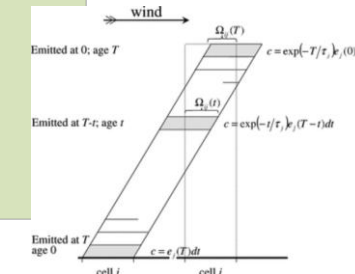
$$\mathbf{x}_i^b = \begin{bmatrix} \mathbf{c}_i^b \\ \mathbf{e}_i^b \end{bmatrix};$$

$$J(x, p) = \underbrace{(\mathbf{x} - \mathbf{x}_b)^T \mathbf{B}^{-1} (\mathbf{x} - \mathbf{x}_b)}_{J_b: \text{background constraint for } \mathbf{x}} + \underbrace{(\mathbf{p} - \mathbf{p}_b)^T \mathbf{B}_p^{-1} (\mathbf{p} - \mathbf{p}_b)}_{J_p: \text{constraint for emission scaling factors}} + \underbrace{\sum_{i=0}^n (\mathbf{y}_i - \mathbf{H}_i[\mathbf{x}_i, \mathbf{p}])^T \mathbf{R}_i^{-1} (\mathbf{y}_i - \mathbf{H}_i[\mathbf{x}_i, \mathbf{p}])}_{J_o: \text{observation constraint}}$$

State control vector + Parameter (e.g. scaling factors)

$$\frac{\partial(V_{NO_x})}{\partial t} = E_{NO_x} + L_{NO_x} + \nabla \cdot (V_{NO_x} \mathbf{w})$$

$$E_{top-down} = E_{apriori} \times \left( \frac{\Omega_{observed}}{\Omega_{model}} \right)$$



- State vector forecast  $\mathbf{e}^f(t_{i+1}) = \mathbf{M}_i[\mathbf{e}^f(t_i)]$  (K1)
- Error cov. forecast  $\mathbf{P}^f(t_{i+1}) = \mathbf{M}_i \mathbf{P}^f(t_i) \mathbf{M}_i^T + \mathbf{Q}(t_i)$  (K2)
- Gain matrix  $\mathbf{K}_i = \mathbf{P}^f(t_i) \mathbf{H}_i^T [\mathbf{H}_i \mathbf{P}^f(t_i) \mathbf{H}_i^T + \mathbf{R}_i]^{-1}$  (KG)
- State vector analysis  $\mathbf{e}^a(t_i) = \mathbf{e}^f(t_i) + \mathbf{K}_i (\mathbf{y}_i - \mathbf{H}_i[\mathbf{e}^f(t_i)])$  (K3)
- Error cov. analysis  $\mathbf{P}^a(t_i) = (\mathbf{I} - \mathbf{K}_i \mathbf{H}_i) \mathbf{P}^f(t_i)$  (K4)

# Correzione dei modelli fotochimici tramite osservazioni satellitari: dall'assimilazione dati all'inversione

Giorgia De Moliner – PhD student

