Operational Data Assimilation for Earth System Models: Challenges and Opportunities

Nicolas Bousserez and the CAMS team

Atmosphere Monitoring

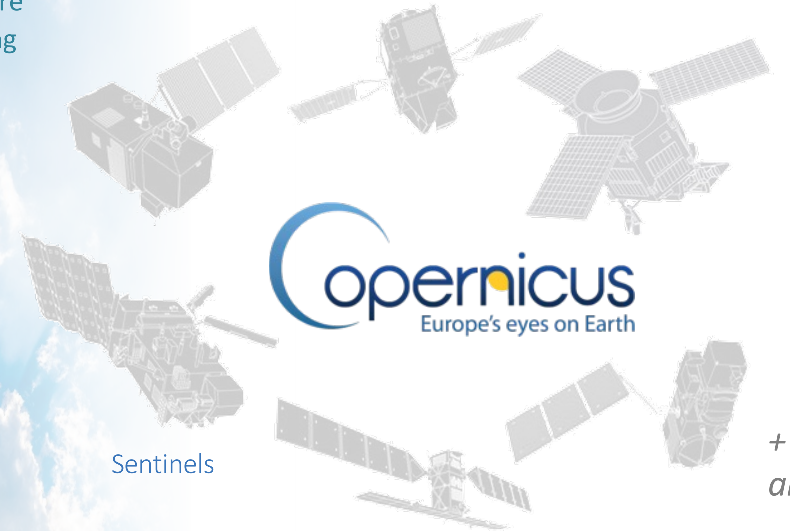
PROGRAMME OF THE EUROPEAN UNION

Copernicus Europe's eyes on Earth

IMPLEMENTED BY ECMWF

Atmosphere Monitoring

COPERNICUS AND ECMWF



Observations combined with models to provide value-added Services

+ many other satellites and non-satellite data

- Atmosphere
- Climate
- Land
- Marine
- Emergency
- Security

Copernicus is the European Union's operational Earth Observation and Monitoring programme, looking at our planet and its environment for the ultimate benefit of everyone.

User-driven with free and unrestricted data access

Service is implemented by ECMWF

ECWMF is contributing to the Service

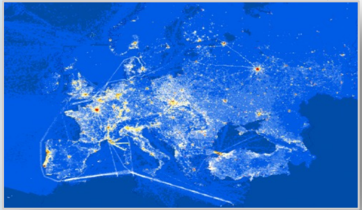
PROGRAMME OF THE EUROPEAN UNION

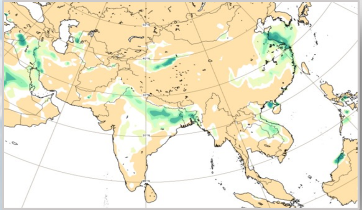
Copernicus Europe's eyes on Earth

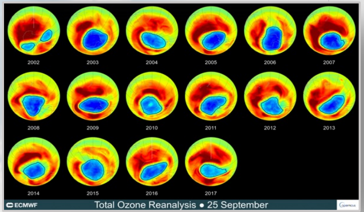
IMPLEMENTED BY ECMWF

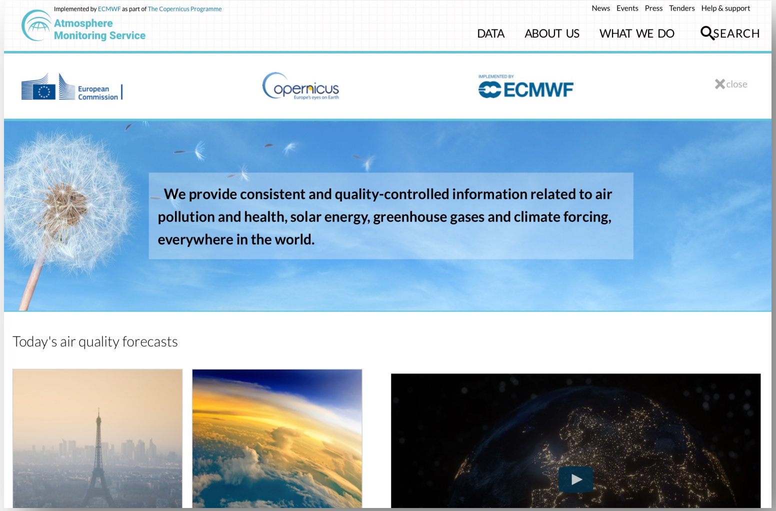
Atmosphere Monitoring

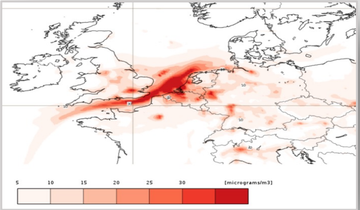
What has the Copernicus Atmosphere Monitoring Service to offer?

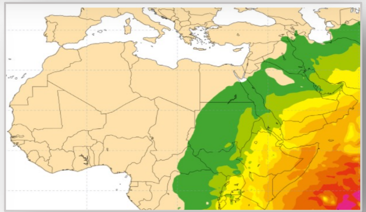












The CAMS portfolio built over the last 15 years includes information products about:

- past, current and near-future (forecasts) global atmospheric composition;
- the ozone layer;
- air quality in Europe;
- emissions and surface fluxes of key pollutants and greenhouse gases;
- solar radiation;
- climate radiative forcing.

Detailed evaluation and quality control information is provided for all the products, most often in the form of quarterly reports.

https://atmosphere.copernicus.eu

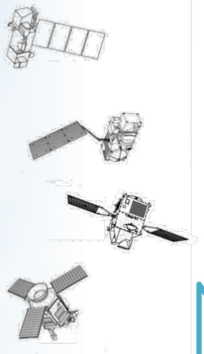
PROGRAMME OF THE EUROPEAN UNION

Copernicus Europe's eyes on Earth

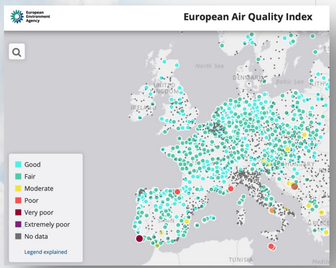
IMPLEMENTED BY ECMWF

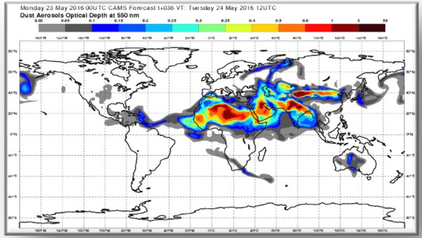
CAMS Information Flow

Atmosphere Monitoring



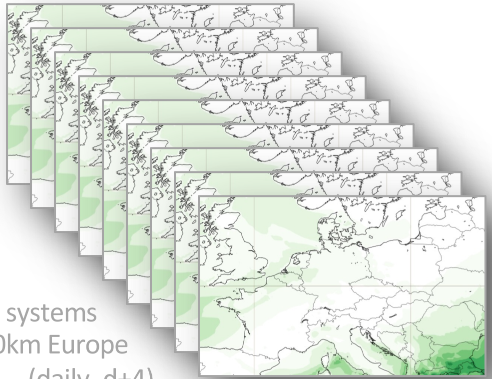
Earth Observation from satellite (>90 instruments) and in-situ (regulatory and research)



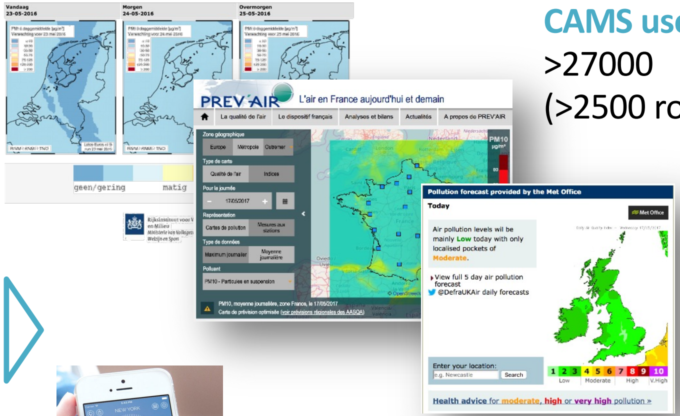


Augmented version of ECMWF IFS
40km (twice daily d+5 forecasts) / 80km (reanalysis)

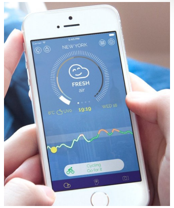
CAMS main operational **data assimilation and modelling systems**



11 systems
10km Europe
(daily, d+4)



CAMS users
>27000
(>2500 routine)



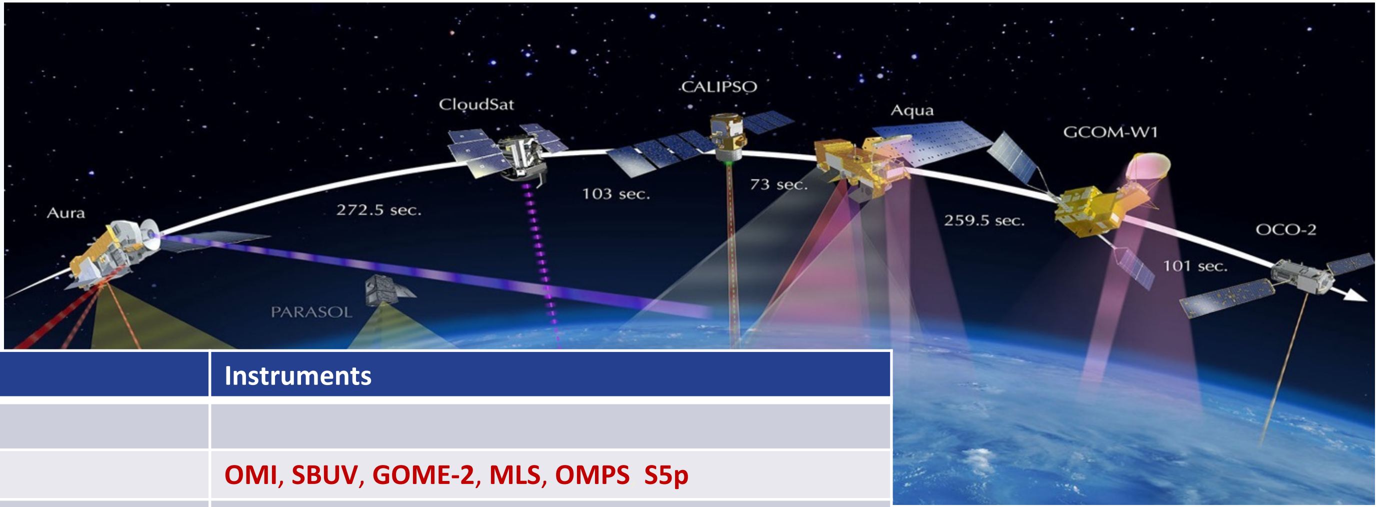
Major multiplication factor
Everyday CAMS data reaches 23M in Europe and 229M worldwide

Windy.com

The Weather Channel

EO satellites used in CAMS

Atmosphere Monitoring



Species	Instruments
Global system	
O_3	OMI, SBUV, GOME-2, MLS, OMPS S5p
CO	IASI, MOPITT, **S5p**
NO_2	OMI, GOME-2, S5p
SO_2	OMI, GOME-2, S5p
Aerosol	MODIS, PMAp, VIIRS, S3
CO_2	GOSAT, **OCO-2**
CH_4	GOSAT, IASI, **S5p**
GFAS fire emissions	MODIS, **SEVIRI***, **VIIRS**, Sentinel-3, GOES-E/W*, HIMAWARI-8*

Assimilated **Monitored** Under test

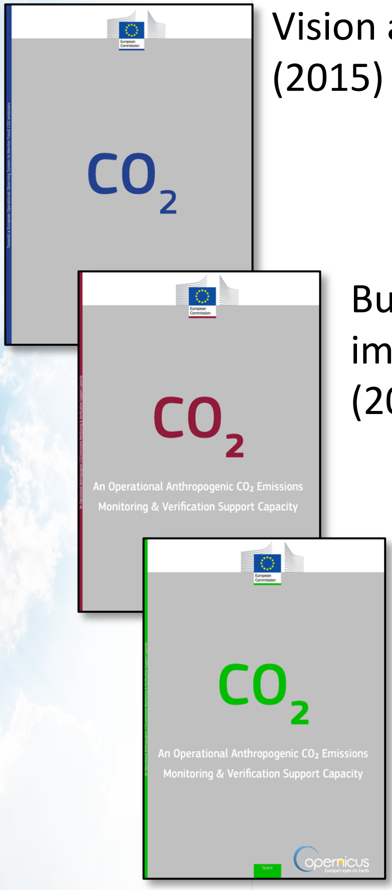
*Geostationary platform

CAMS uses Earth Observation data from many satellites for atmospheric composition and weather (not reported on this table).

PROGRAMME OF THE EUROPEAN UNION Copernicus Europe's eyes on Earth IMPLEMENTED BY ECMWF

Emission Monitoring: From Vision to Implementation

Atmosphere Monitoring



Vision and strategy (2015)

Building blocks and implementation (2017)

Role and requirements for in-situ data (2019)

- New monitoring needs have emerged in the context of the Paris agreement to support the parties with their Nationally Determined Contribution (NDC) and the Global Stocktake (GST).
- The European Commission tasked a group of experts to develop a vision for and provide advice on implementation of a Copernicus CO_2 emission monitoring service.
- ECMWF was entrusted by the European Commission to build this new operational CO_2 Monitoring and Verification System (CO2MVS).

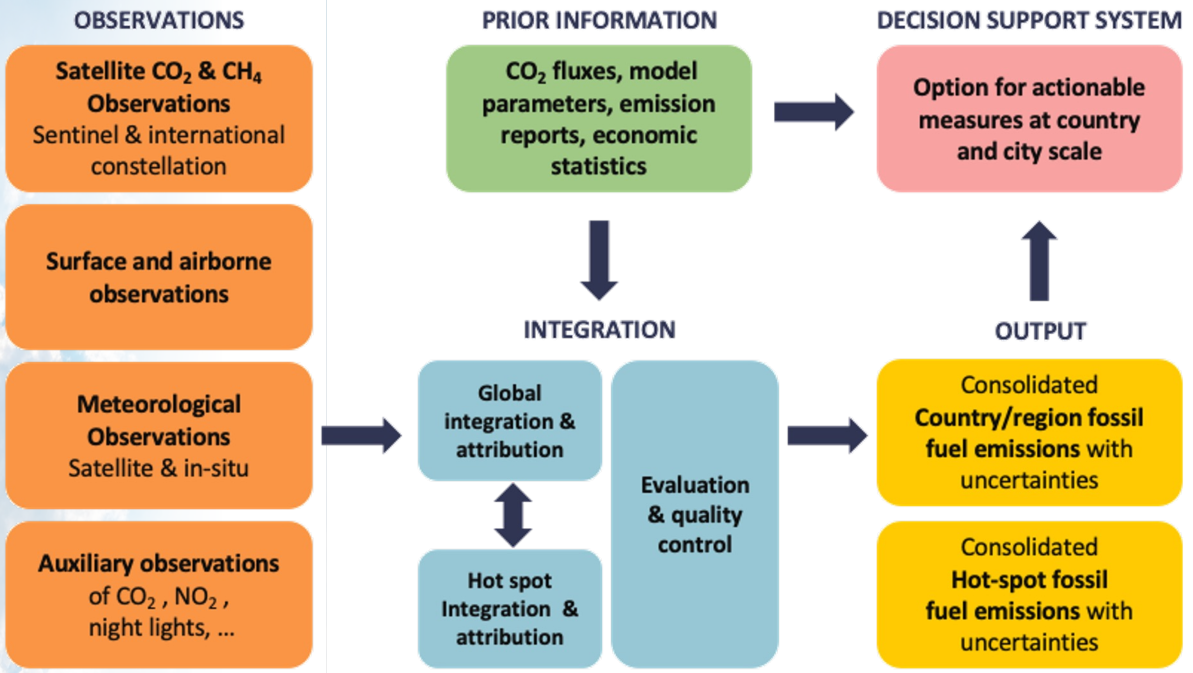
PROGRAMME OF THE EUROPEAN UNION

Copernicus Europe's eyes on Earth

IMPLEMENTED BY ECMWF

Atmosphere Monitoring

A new Copernicus Emission Monitoring Service



Atmosphere Monitoring Service

atmosphere.copernicus.eu

- An integrated system approach based on experience in NWP and air quality monitoring & forecasting.
- Same system (in potentially different configurations) for greenhouse gases and atmospheric pollutants.

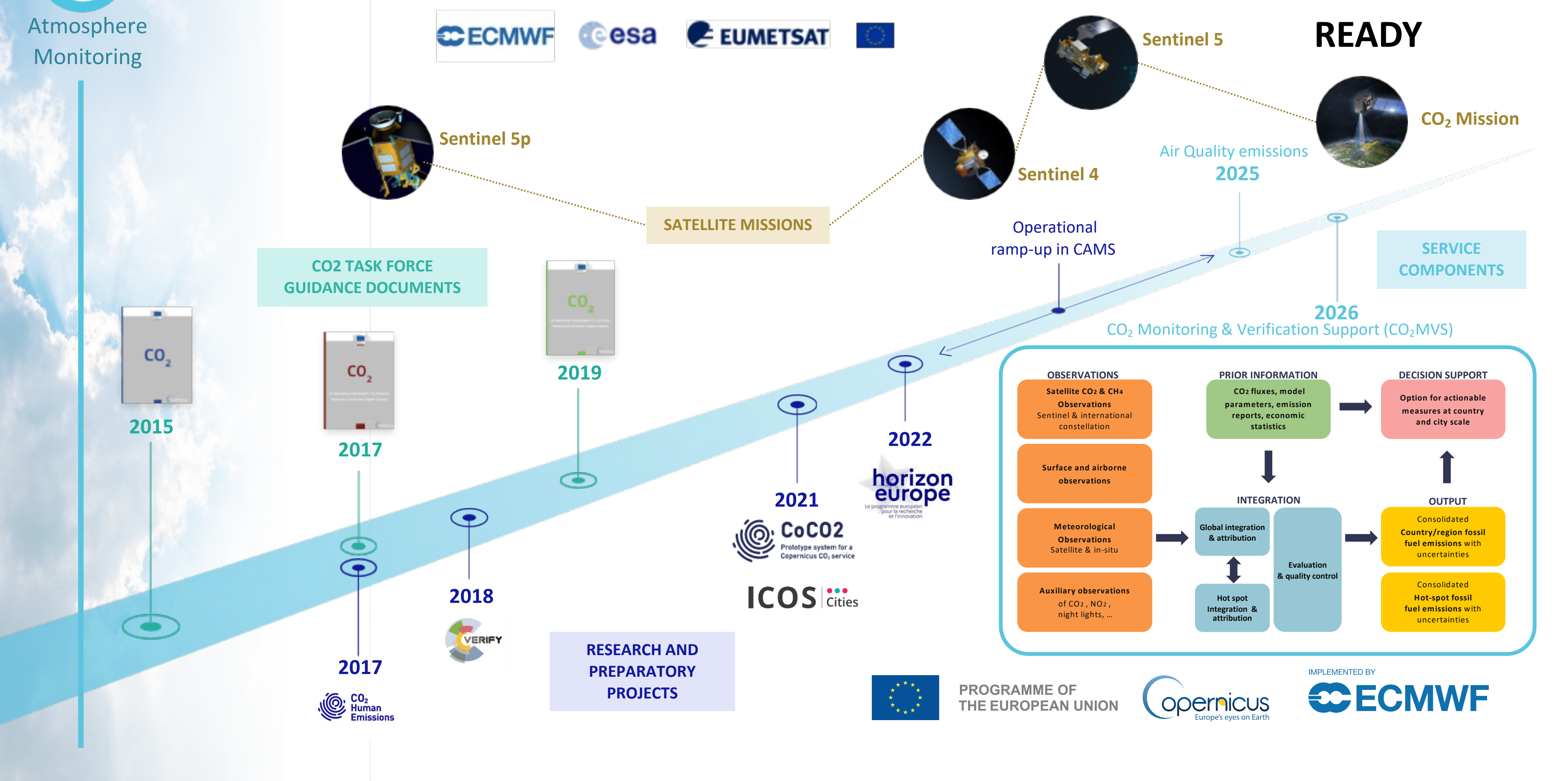
PROGRAMME OF THE EUROPEAN UNION

Copernicus Europe's eyes on Earth

IMPLEMENTED BY ECMWF

esa EUMETSAT

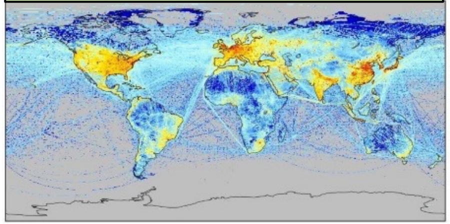
Timeline of the CAMS Emissions Services



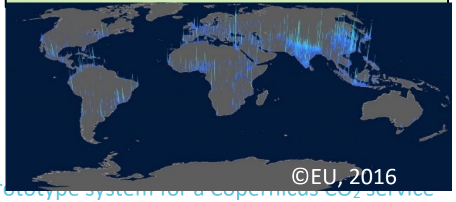
The IFS global inversion system

INPUT DATASETS

EMISSION INVENTORIES WITH TEMPORAL/VERTICAL PROFILES & UNCERTAINTIES (JRC EDGAR,TNO/BSC, CAMS81)

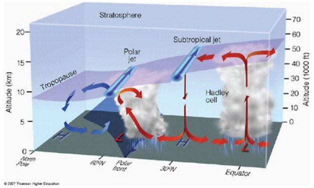


VEGETATION & URBAN MAPS (ESA-CCI, JRC GHSL) OCEAN FLUXES (CMEMS)

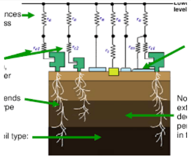


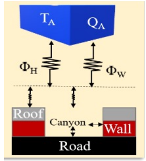
IFS FORECAST MODEL & DATA ASSIMILATION

IFS ATMOSPHERIC TRANSPORT

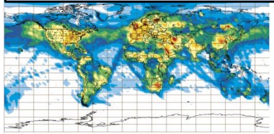


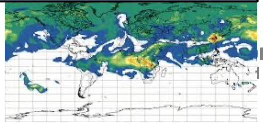
URBAN & VEGETATION MODEL, LAND SURFACE DATA ASSIMILATION



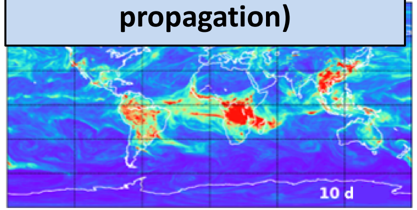


CAMS REACTIVE SPECIES (NOx, CO, CH4)

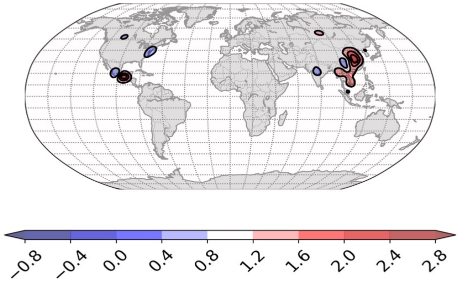




ENSEMBLE APPROACH (uncertainty estimation & propagation)



4D-VAR ATMOSPHERIC ANALYSIS & INVERSION CAPABILITY



Multi-species 4D-Variational inversion

$$J(\mathbf{x},\mathbf{p}) = (\mathbf{x}-\mathbf{x}_b)^T\mathbf{B}_\mathbf{x}^{-1}(\mathbf{x}-\mathbf{x}_b)+(\mathbf{p}-\mathbf{p}_b)^T\mathbf{B}_\mathbf{p}^{-1}(\mathbf{p}-\mathbf{p}_b)+(\mathbf{y}-h(\mathbf{x},\mathbf{p}))^T\mathbf{R}^{-1}(\mathbf{y}-h(\mathbf{x},\mathbf{p}))$$

state (prognostic) — parameter (e.g., emission scaling factors) — observations (meteorology, atmospheric composition)

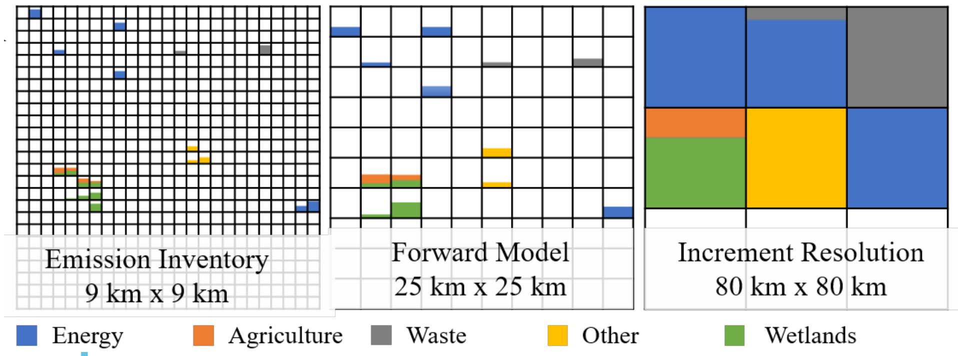
- <u>Characteristics of current system:</u>
  - **Online system**: joint meteorology & chemistry state/fluxes 4D-Var optimisation
  - 12-hour or 24-hour window
  - Emissions: CO_2, CH_4, NO_x, CO
  - Biogenic CO_2 fluxes (GPP and respiration): process-based online prior
  - Observations: OMI NO_2; TROPOMI NO_2, CO, CH_4 ; IASI CH_4; GOSAT CO_2, CH_4; OCO-2 & OCO-3 CO_2
  - **B** model: spatial error correlations, cross-species correlations
- Tangent linear and adjoint models of simplified chemistry mechanism
- Co-emitter prior correlations (CO_2, CO, NO_x): enables constraints on anthropogenic CO_2 emissions from NO_2 observations
- Posterior error covariance estimation based on ensemble of data assimilation (EDA) approach (i.e., Monte-Carlo)
- <u>Limitation</u> : optimization of GHG fluxes requires much longer assimilation window (~months to years)→ building a long-window hybrid ensemble-variational system

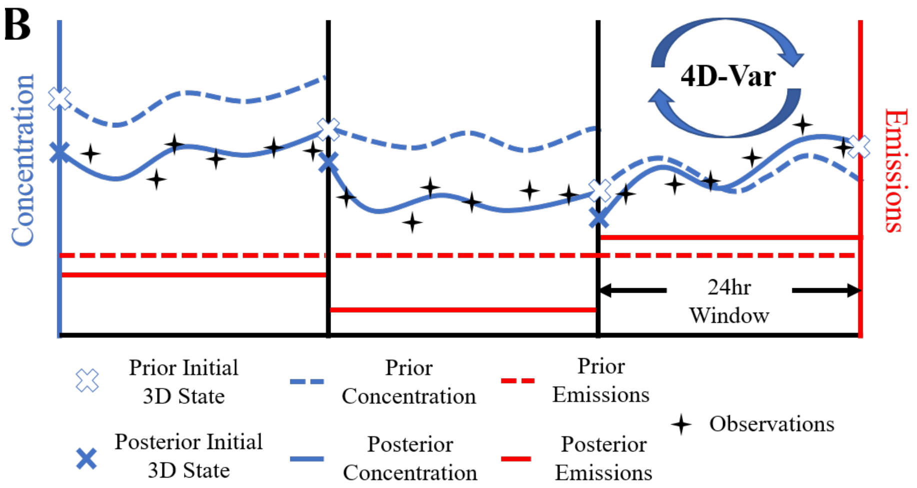
PROGRAMME OF THE EUROPEAN UNION — opernicus Europe's eyes on Earth — IMPLEMENTED BY ECMWF

First application: CH_4 source inversion

- Forward model at Tco399 (~25km), increment at Tl255 (~80km), 137 levels
- CAMS prior emissions
- Prior error derived from literature, adjusted based on best fit of inversion against independent observations
- Daily posterior fluxes for 7 sectors (4 anthropogenic)
- Observations: XCH_4 GOSAT, IASI and TROPOMI
- Case studies selected based on existing studies using well tested systems
- 3D state initialised from operational CAMS inversion product

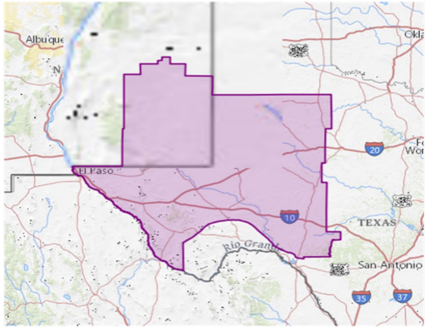
(McNorton et al., 2022)



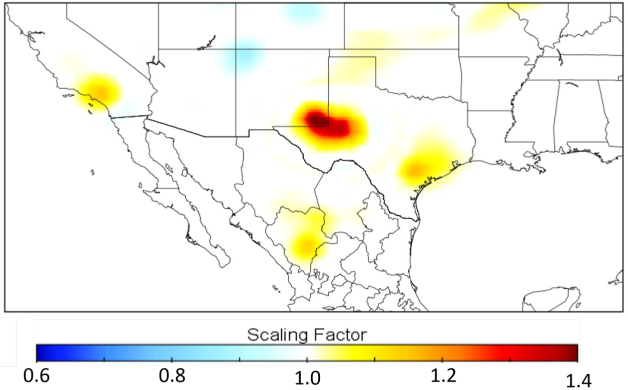


Inversion of methane emissions from oil & gas fields over the US

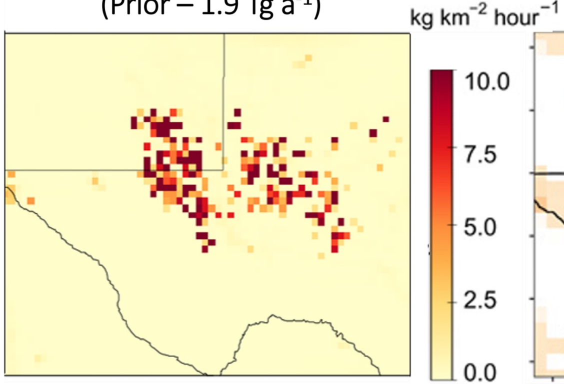
The Permian Basin



Analysis Emissions of Permian Basin (03/01/2019)



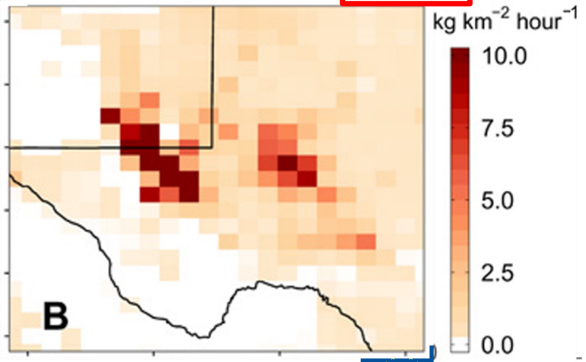
IFS Posterior – 2.5 Tg a^{-1}
(Prior – 1.9 Tg a^{-1})



This study

- IFS 4D-Var inversion
- TROPOMI, GOSAT, IASI observations

Zhang et al. Posterior – 2.9 Tg a^{-1}

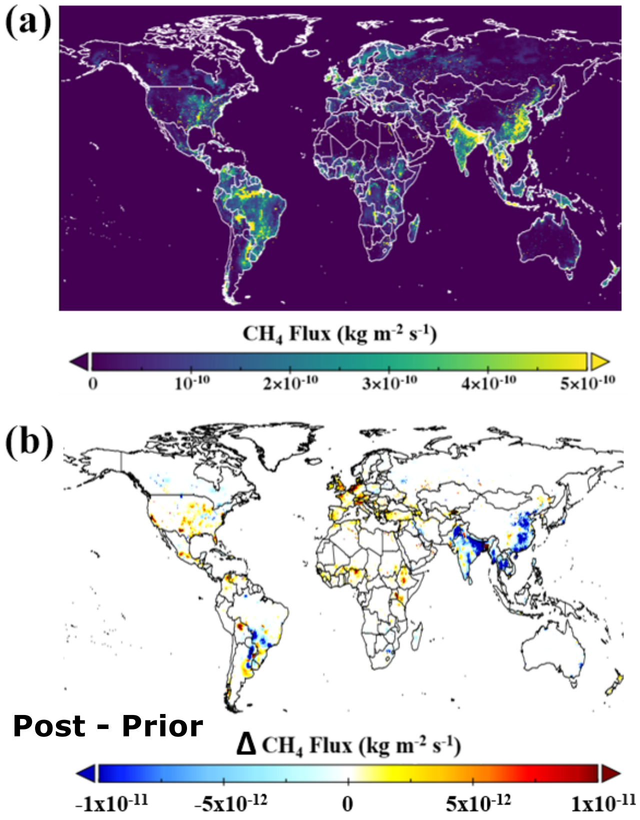


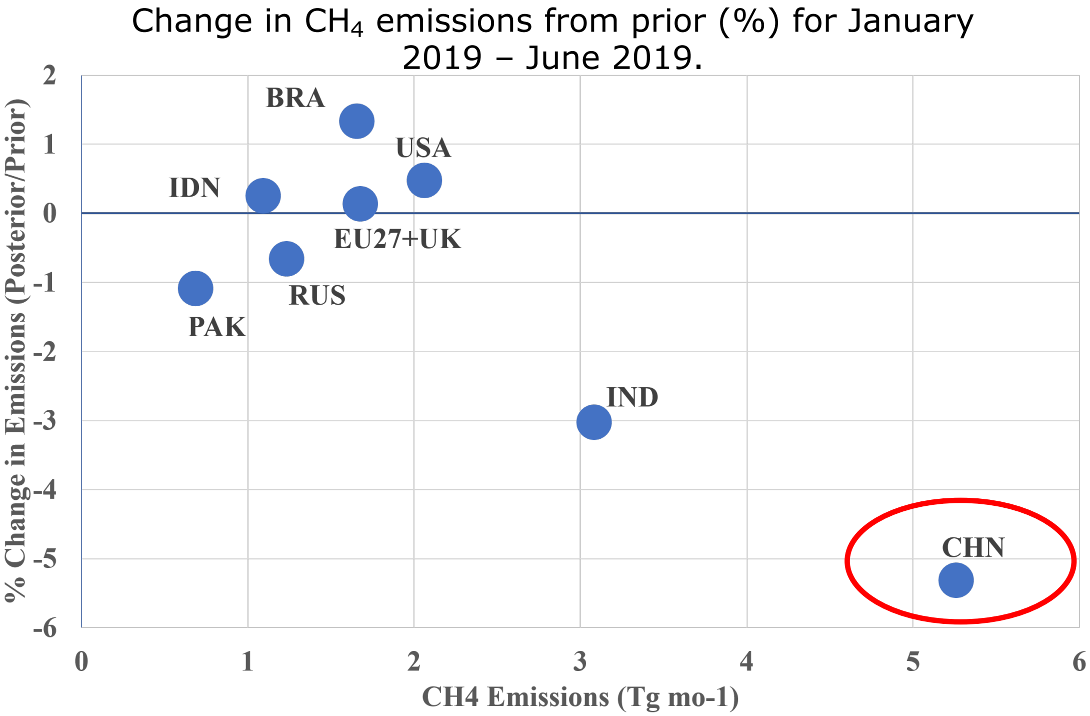
Zhang et al., 2020

- GEOS-CHEM 0.5°
- TROPOMI observations

- The IFS inversion results are consistent with previous findings, showing an underestimation of the prior CH_4 emissions over the Permian Basin (McNorton et al., 2022).
- Posterior emission correction in agreement with previous top-down inversion study (Zhang et al., 2020)

Global posterior CH_4 budget for 2019





- ➢In agreement with known overestimation in bottom-up inventories over China (e.g., Cheewaphongphan et al., 2019)
- ➢ Posterior generally in closer agreement with previous top-down estimates (e.g., Deng et al., 2022)

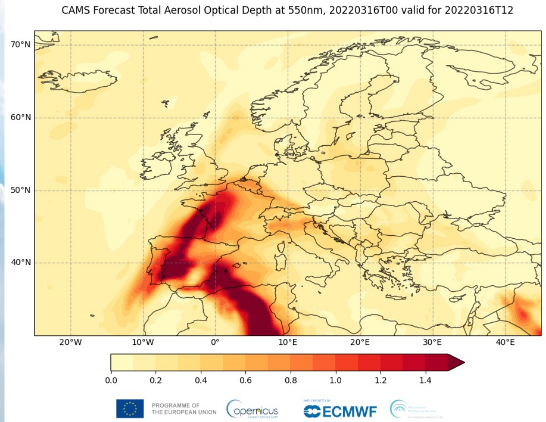
Benefits of Integrated Earth System Data Assimilation

- Physically consistent observation-based estimation of the state of the Earth system:
  - Modeling of interactions between all processes of the Earth system.
  - Online modeling of prior covariances between all variables/parameters in Bayesian inversion.
- Examples:
  - Aerosol radiative effect feedbacks.
  - Atmospheric tracers observations can constrain the wind fields.
  - Flux inversion: transport errors (including correlations) from meteorological uncertainties implicitly accounted for.
  - Impact of meteorology on chemical fluxes (wetland CH_4 emissions, anthropogenic CO_2 emissions from energy sector, etc.)

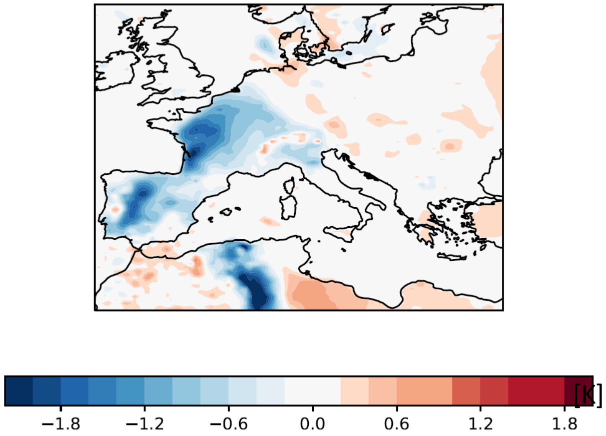
Atmospheric composition impacts on NWP

Atmosphere Monitoring

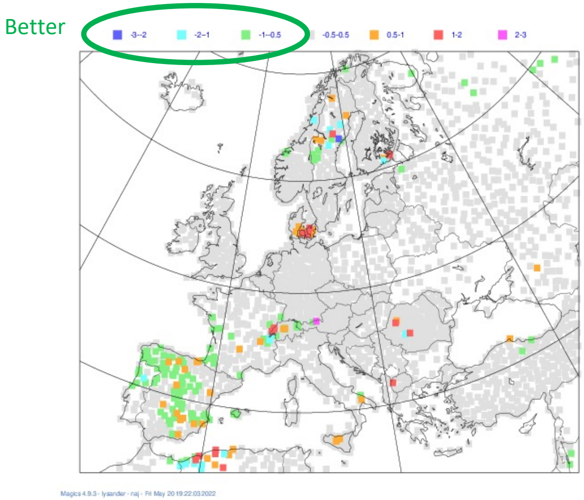
- IFS includes prognostic aerosols and ozone which are interactive with the model radiation scheme.
- Control runs using climatological (i.e., non-interactive) aerosols allow evaluation of impacts on NWP fields, e.g., 2m temperature, during pollution episodes.



CAMS operational total aerosol optical depth forecast Initialized 00 UTC and valid for 12 UTC on 16 March 2022



12-15 UTC mean 2m temperature difference (prognostic – climatological aerosol)

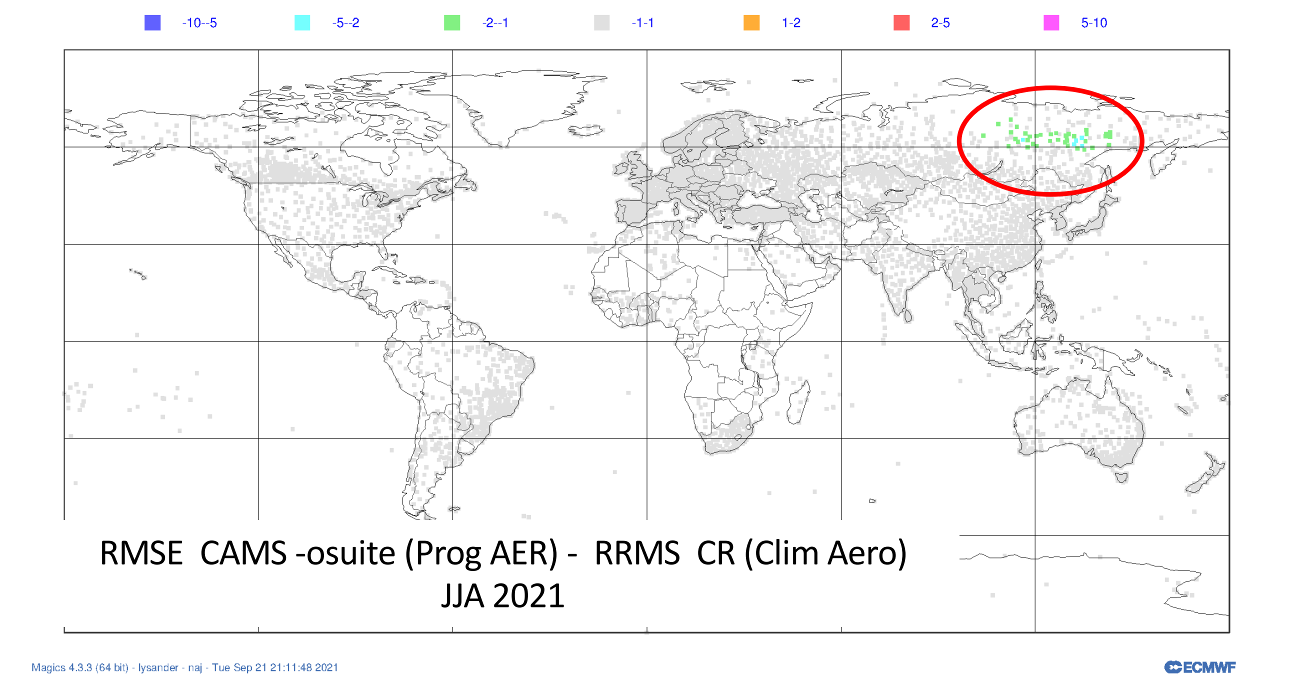


Mean 2m temperature absolute error difference (prognostic / CAMS – climatological aerosol)

- Including prognostic aerosols generally improves 2m temperature errors, e.g., shown across SW Europe during March 2022 Saharan dust episode.
- Similarly for episode in February-March 2021: https://www.ecmwf.int/en/newsletter/168/news/saharan-dust-events-spring-2021

Impact of Artic wildfires on 2m temperature forecasts (JJA 2021)

Atmosphere Monitoring



- Using prognostic aerosols leads to decrease in 2m temperature RMSE against synop observations

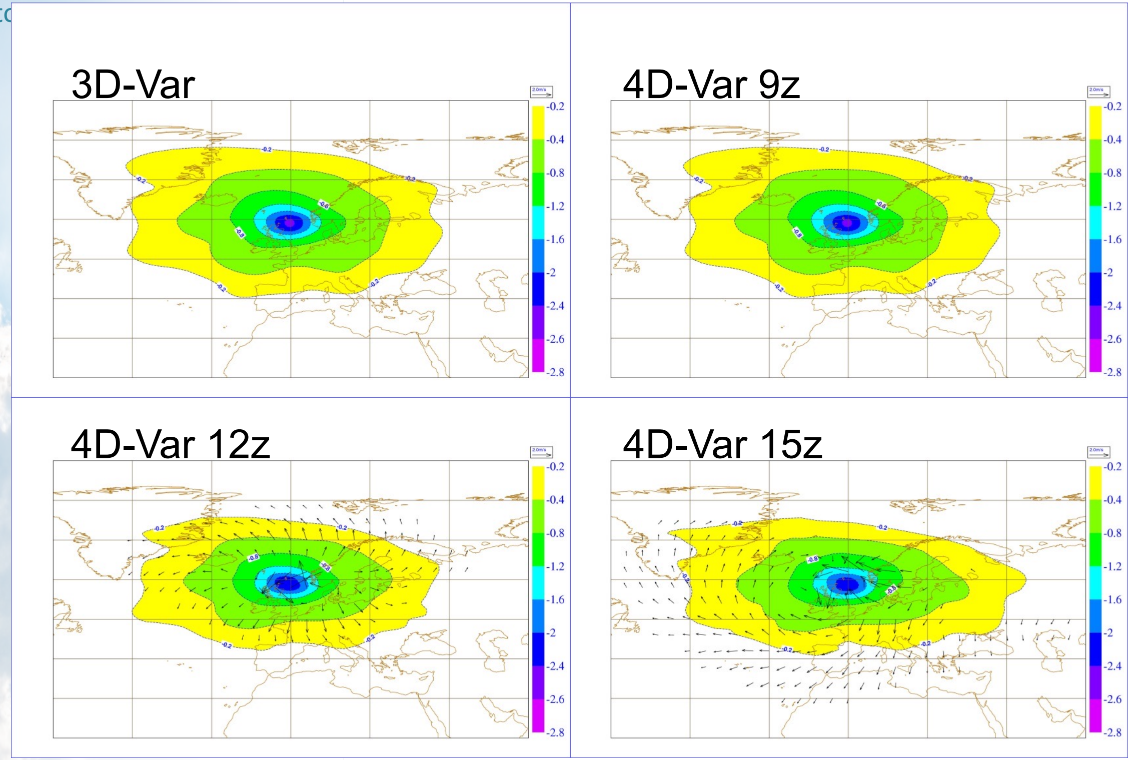
PROGRAMME OF THE EUROPEAN UNION

Copernicus Europe's eyes on Earth

IMPLEMENTED BY ECMWF

Credit: Johannes Flemming

Ozone and wind increments



Level 20,
≈ 30 hPa

- 6h assimilation window
- Observation at T0: 4D-Var = 3D-Var
- Observation at T3: wind increments
- Observation at T6: wind increments

Single observation experiments

Meteorology impact on prior emissions

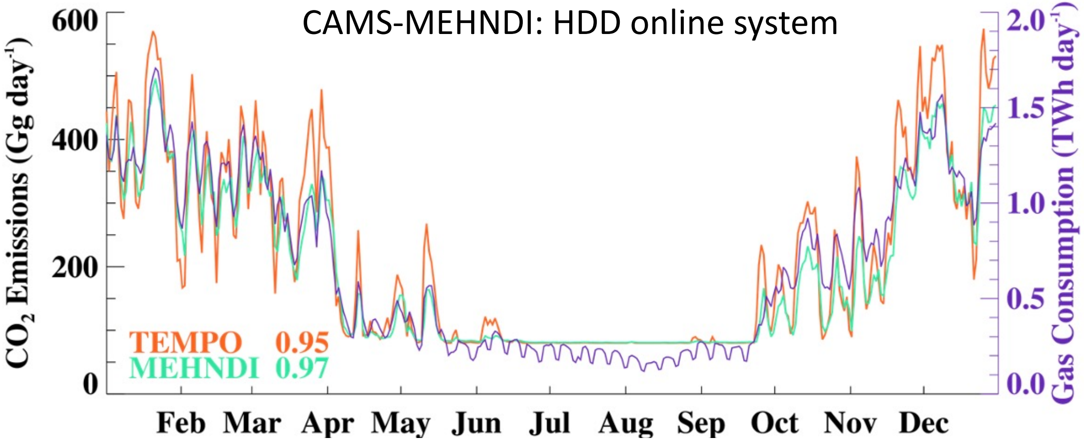
<u>Use of a urban tile combined with a Heating Degree Day (HDD) model:</u>

$$\text{Flux} = U_{cover}\,\gamma f(T_{urban})$$

$$f(T_{urban}) = \max(15.5 - Tsoil(lev\ 1), 1)$$

- γ, is a national scaling factor based on annual residential heating.
- U_{cover} is the urban cover.
- $f(T_{urban})$ is the heating degree day function.

CAMS-TEMPO: HDD model offline
CAMS-MEHNDI: HDD online system



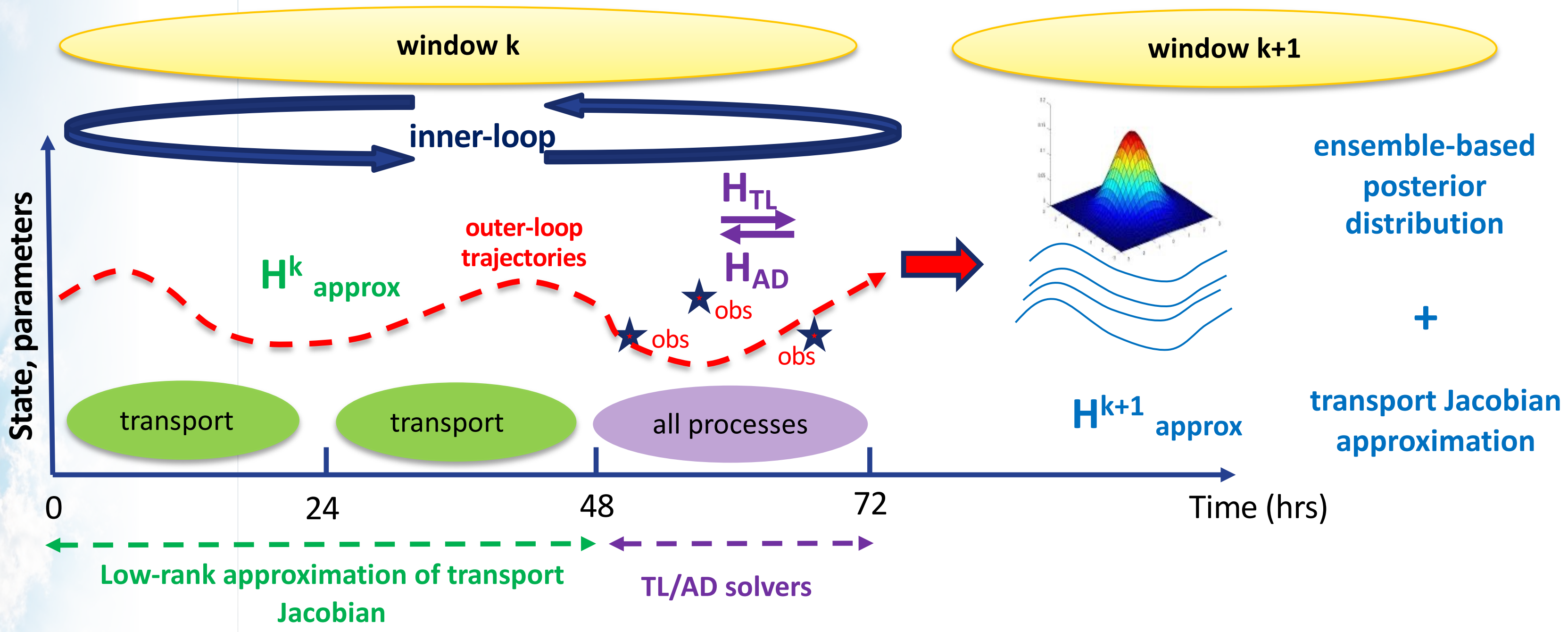
Credit: Joe McNorton

Challenges of Integrated Earth System Data Assimilation

- High computational cost:
  - Requires efficient algorithms to meet operational time constraints.
  - Limits resolution capabilities.
- Non-linearities:
  - Short-window 4D-Var to avoid convergence issues (e.g., multiple minima) →incompatible with long-lived tracers inversion problems.
  - Incremental 4D-Var tangent-linear approximation might not always hold when going to higher resolutions.

Atmosphere Monitoring

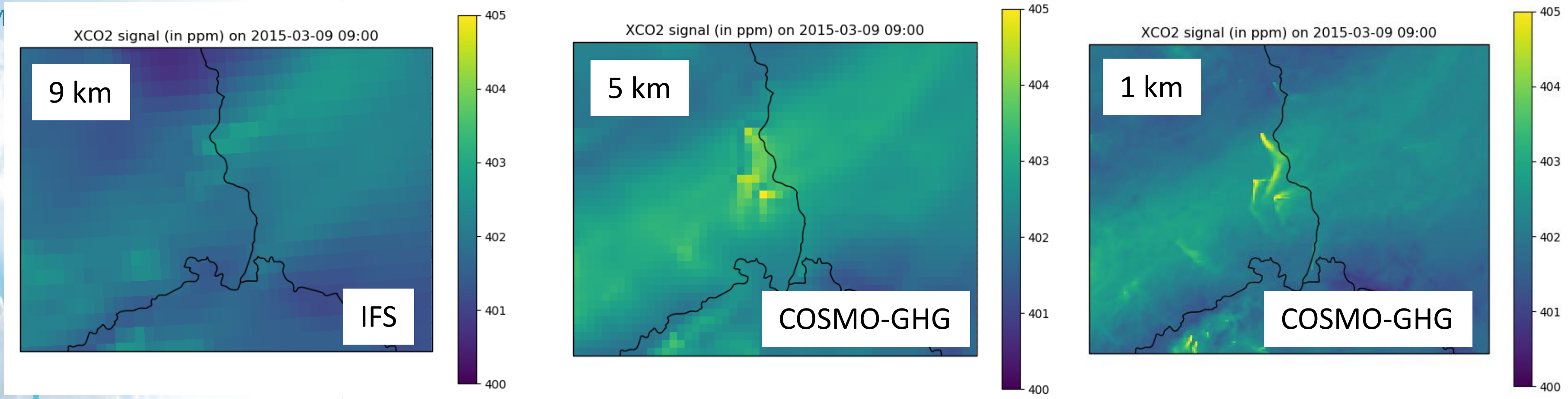
Extended 4D-Var window for GHG inversion



- Tangent-linear/adjoint models used for short-window containing current observations.
- Low-rank approximation of transport used for previous days.

Importance of resolution in the source inversion problem

Power stations & CO_2 emissions (Berlin area)



- Current computational cost limits spatial resolution of global inversion (currently ~ 9 km for IFS forward model, ~ 80 km for TL/AD (i.e., increments)).
- IFS spatial resolution planned to eventually reach 2 km to 1 km within 10 years.
- In the meantime, regional and local inversion systems with higher transport resolution provide necessary information for accurate estimation of emissions.
- Strong benefits from integrating regional/local inversions information into global inversion system.

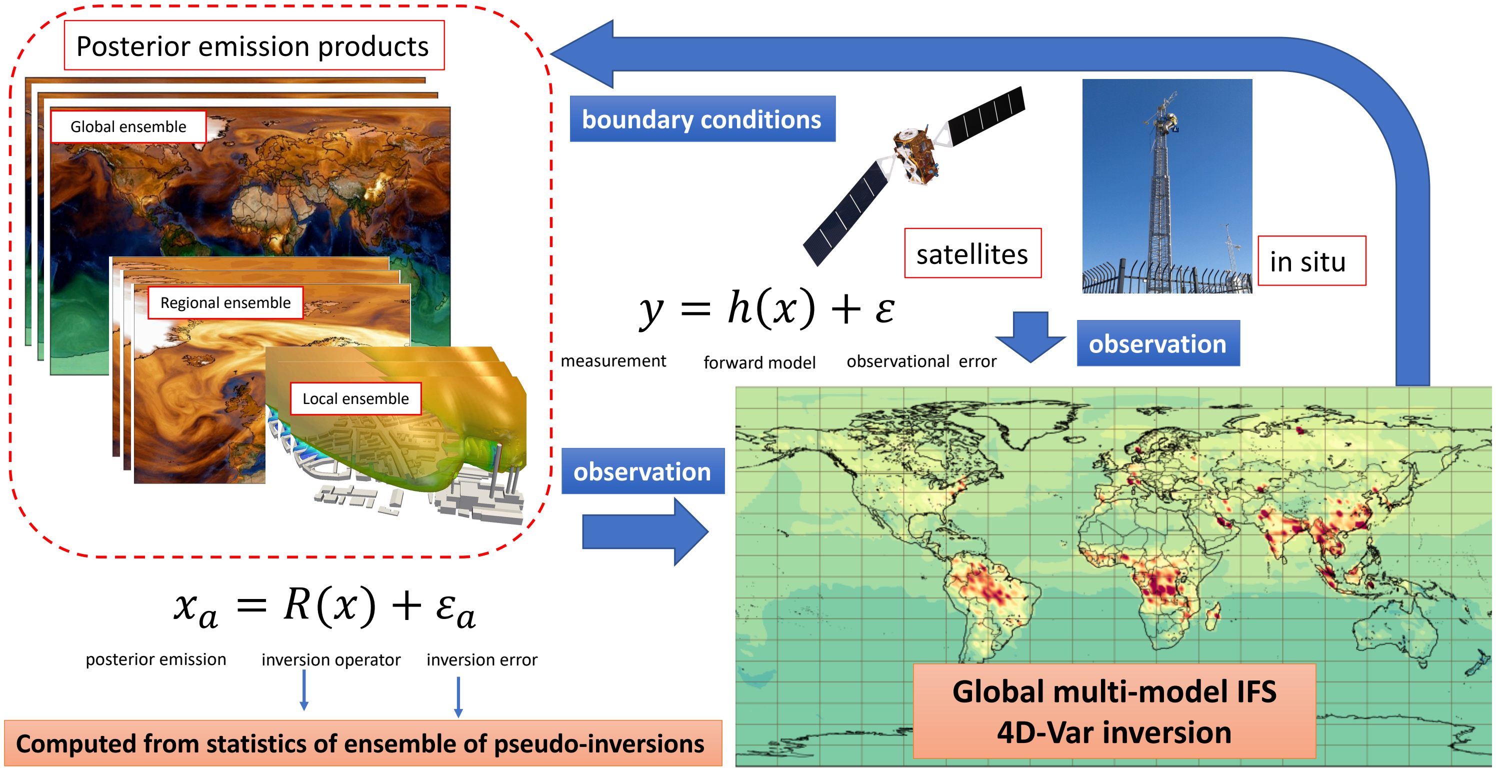
PROGRAMME OF THE EUROPEAN UNION

IMPLEMENTED BY ECMWF

Source: CHE project report

A multi-scale, multi-species, multi-model approach

Multi-model multi-scale approach



PROGRAMME OF THE EUROPEAN UNION

IMPLEMENTED BY

Conclusion and perspectives

- Recent developments in data assimilation for Earth system models open new possibilities for accurate estimation and understanding of the state of the Earth system.
- High societal impact and visibility of current GHG flux estimation projects→new opportunities for funding and collaborations between research groups worldwide.
- ECMWF is undertaking significant development steps towards building a comprehensive atmospheric composition data assimilation system integrating both state and flux optimisation.
- Characteristics of the new system will include:
  - An extended 4D-Var window to accommodate long-lived tracers (CO_2, CH_4, N_2O).
  - Joint optimisation of tracers emissions including prior error correlations to enhance observational constraints (e.g., of CO and NO_2 observations on CO_2 emissions).
- Operational **global Earth system models** can leverage information from higher resolution **limited area models** by assimilating those products as observations.
- Transformative approaches are required to meet both scientific and operational constraints (e.g., machine learning surrogates for chemical models, fast optimisation algorithms using parallelized randomized matrix decomposition, etc.)