Data assimilation of atmospheric composition

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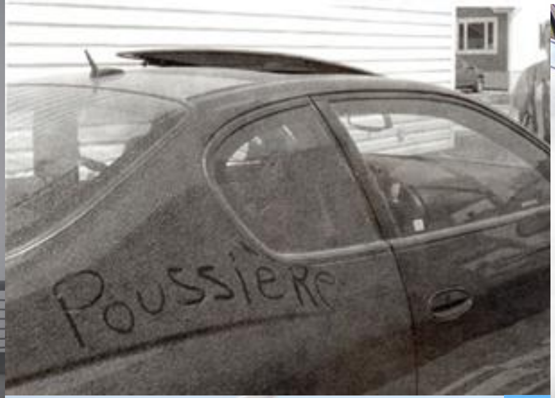
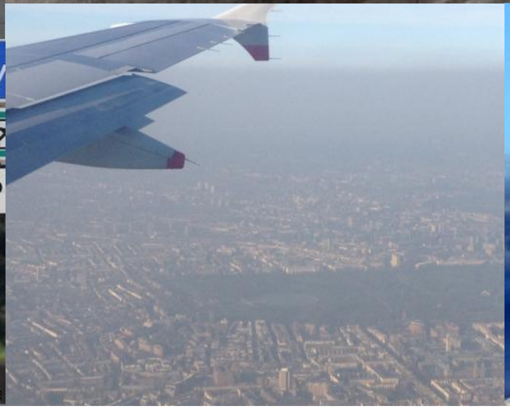
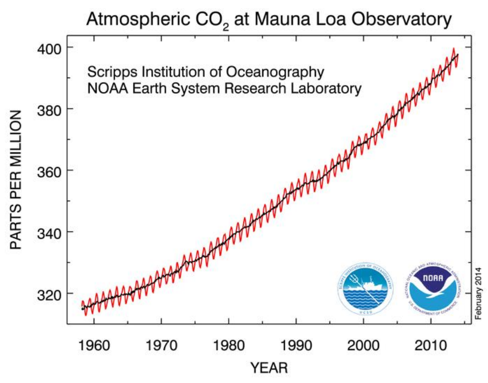
Why atmospheric composition at an operational weather prediction centre?

- Poor air quality is a major public health issue in many countries.
- Local authorities need accurate and timely information to implement effective air pollution mitigation measures.
- Accurate air quality forecasts require accurate transport models.
- Can leverage sophisticated data acquisition infrastructures implemented at operational weather prediction centers.
- Atmospheric composition also impacts the weather and forecasts.

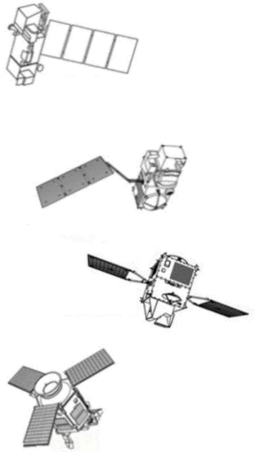




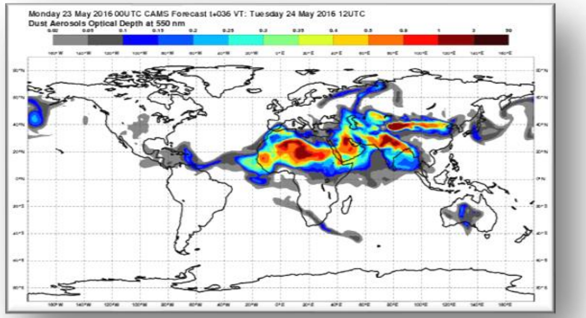


Copernicus Atmosphere Monitoring Service

Atmosphere Monitoring Service
atmosphere.copernicus.eu

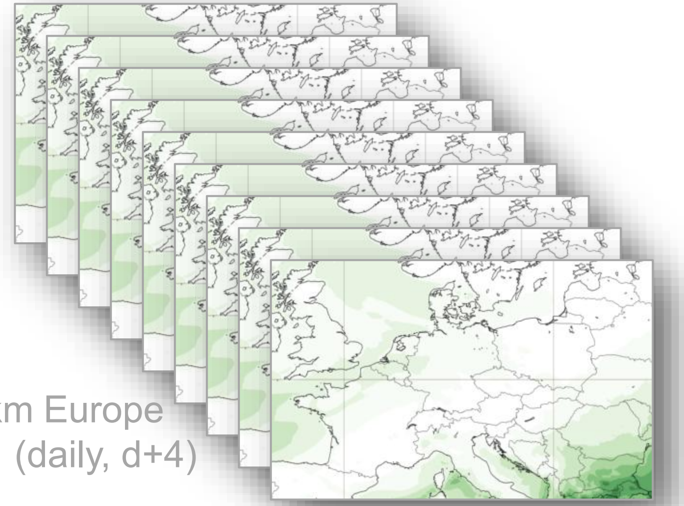


Earth Observation from satellite (>80 instruments) and in-situ (regulatory and research)



40km Globe (twice daily, d+5)

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



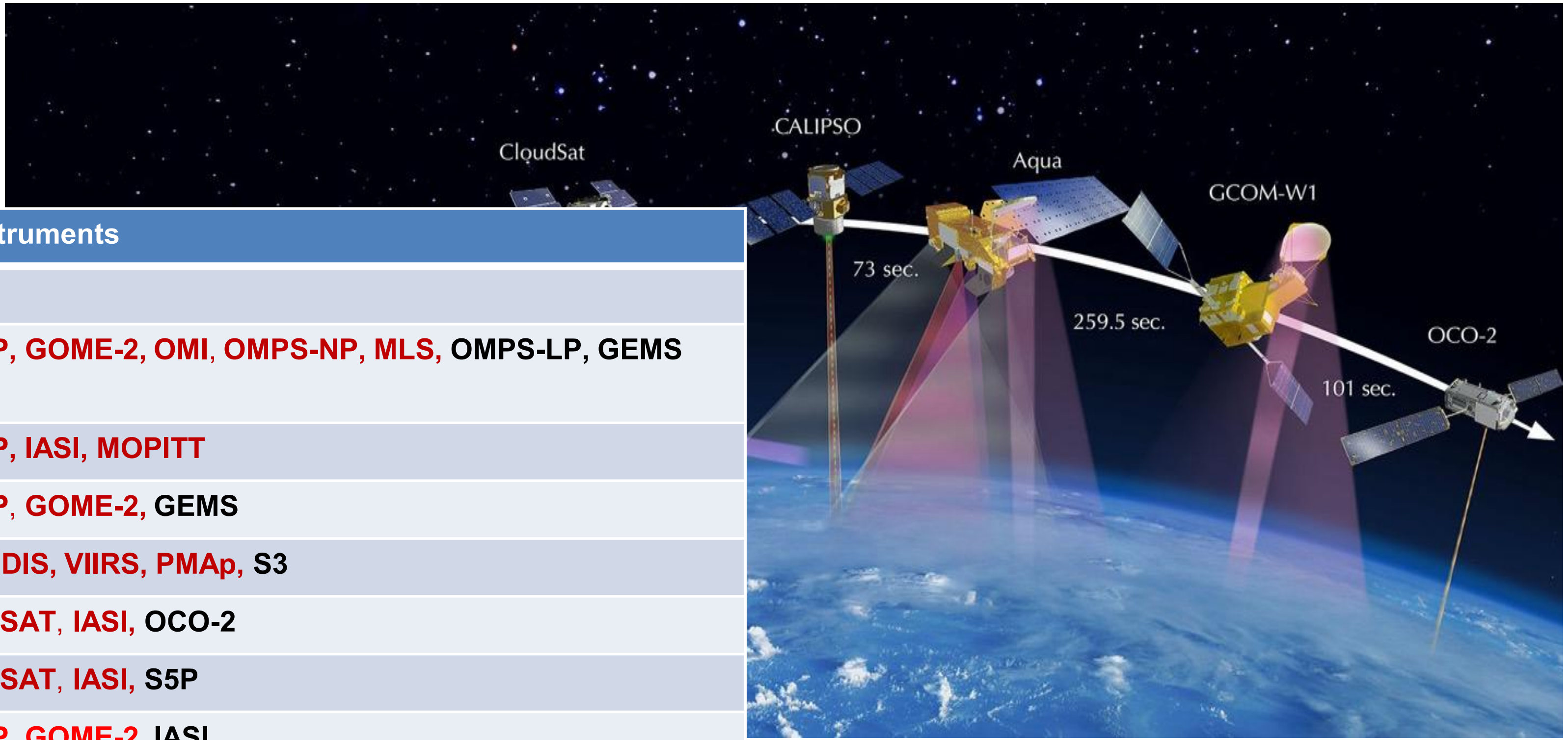
10km Europe (daily, d+4)

CAMS users
>22,500
(>2600 routine)

ECMWF EUROPEAN CENTRE FOR MEDIUM-RANGE WEATHER FORECASTS

AC observations used in CAMS global

Species	Instruments
CAMS NRT	
O_3	S5P, GOME-2, OMI, OMPS-NP, MLS, OMPS-LP, GEMS
CO	S5P, IASI, MOPITT
NO_2	S5P, GOME-2, GEMS
Aerosol	MODIS, VIIRS, PMAp, S3
CO_2	GOSAT, IASI, OCO-2
CH_4	GOSAT, IASI, S5P
SO_2 (volcanic)	S5P, GOME-2, IASI
SO2 (anthropogenic)	S5P
HCHO	S5P
GFAS fire emissions	MODIS, VIIRS, GOES, S3



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

---- Used
---- Undergoing testing

Data assimilation methodology for atmospheric composition

Data Assimilation Methodology

Data assimilation for atmospheric composition is in principle no different from NWP data assimilation

Analysis: x that minimizes cost function

$$J(x) = \underbrace{(x - x_b)^T B^{-1} (x - x_b)}_{J_b \text{ Background term}} + \underbrace{\sum_{i=0}^{n} (y_i - H_i[x_i])^T R_i^{-1} (y_i - H_i[x_i])}_{J_o \text{ Observation term}}$$

x: control vector
x_b: model background (short forecast)
B: Background error covariance matrix
y: Observations
H[x]: Model equivalent of observations
R: Observation error covariance matrix

- **Strong constraint 4D-Var** assumes perfect model over assimilation period
- Weak constraint 4D-Var includes a model error term – developed for O3 and H2O as part of HE CAMEO project

Data Assimilation Methodology

Data assimilation for atmospheric composition is in principle no different from NWP data assimilation

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$$J(x) = (x \quad) + \sum_{i=0}^{n} (y_i - H_i[x_i])^T R_i^{-1} (y_i - H_i[x_i])$$

Control variables

NWP

vorticity
divergence
temperature
surface pressure (logarithm)
specific humidity

Atmospheric Composition

ozone
carbon monoxide
nitrogen dioxide
formaldehyde
sulphur dioxide

carbon dioxide
methane

aerosol mixing ratio

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Atmospheric Composition models

$$x_i = M_{0\to i}(x)$$

Chemical module

GHG module

Aerosol module

Data Assimilation Methodology

Data assimilation for atmospheric composition is in principle no different from NWP data assimilation

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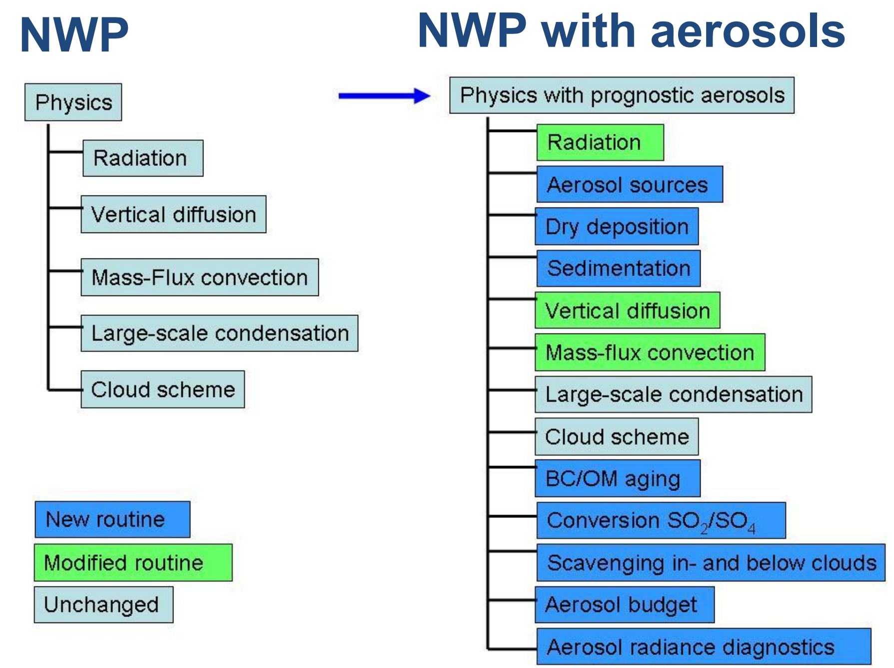


Morcrette et al. 2009, *JGR*, **114**, doi:10.1029/2008JD011235

Incremental 4D-Var

$$\text{Min } J \iff \nabla_{\delta x_0} J = \mathbf{B}^{-1}\,\delta x_0 + \sum_{i=0}^{n} \boldsymbol{M}'^{T}\, \boldsymbol{H}_i^{T} \boldsymbol{R}_i^{-1} (\boldsymbol{H}_i \boldsymbol{M}'_i[\delta x_0] - d_i) = 0$$

Adjoint

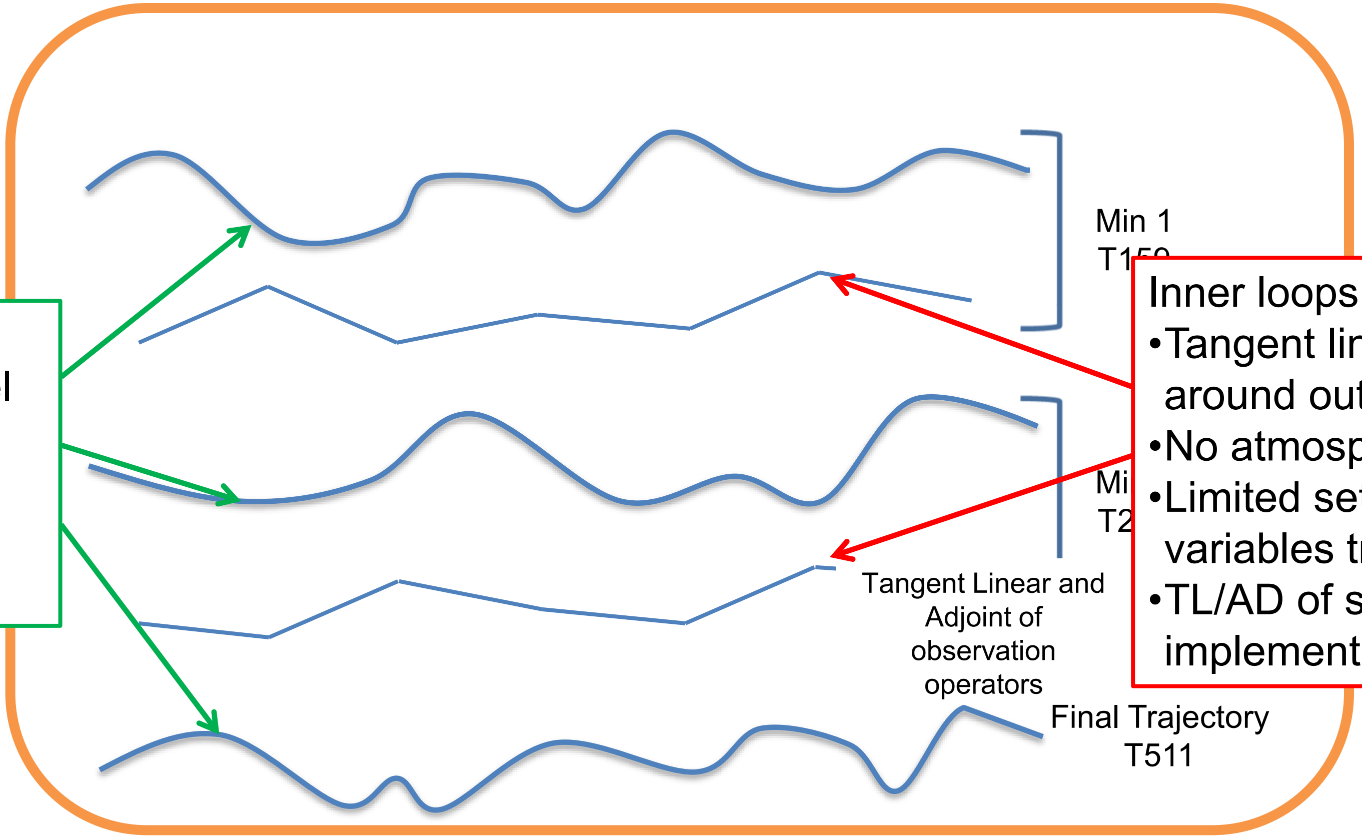
Tangent linear

$d_i = y_i - H_i x_b(t_i)$

Full model

We calculate the gradient of the cost function to find its minimum

Outer loops
- Full non-linear NWP model
- Full atmospheric composition models
- Full set of atmospheric composition variables



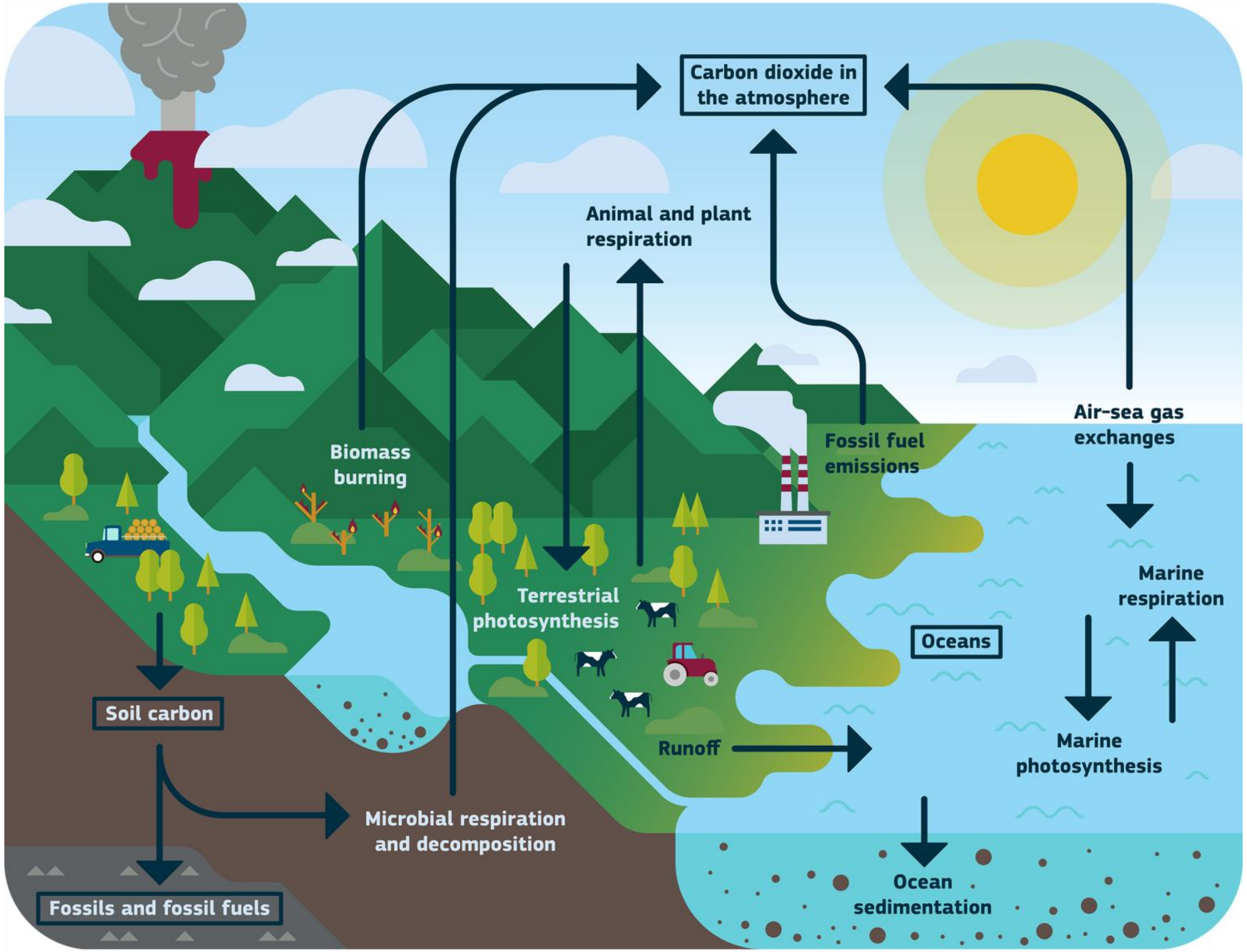
Inner loops
- Tangent linear NWP model linearised around outer-loop trajectory
- No atmospheric composition model
- Limited set of atmospheric composition variables treated as tracers
- TL/AD of simple NO2 chemistry now implemented

Increment

$\delta x = x_a - x_b$

Challenges for Atmospheric Composition Data Assimilation

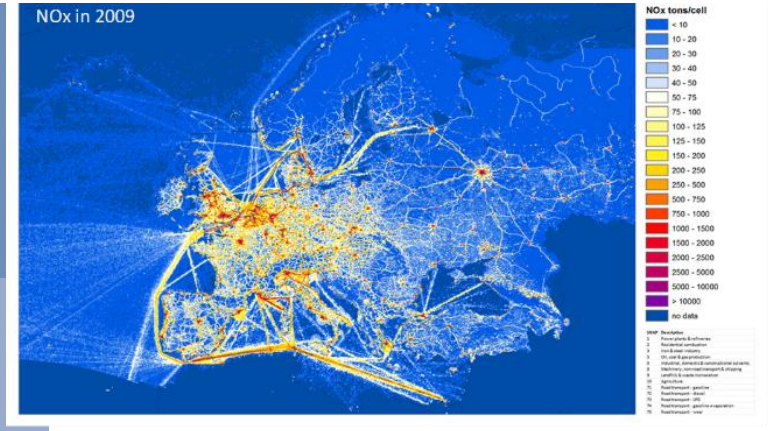
1. Initial versus Boundary problem



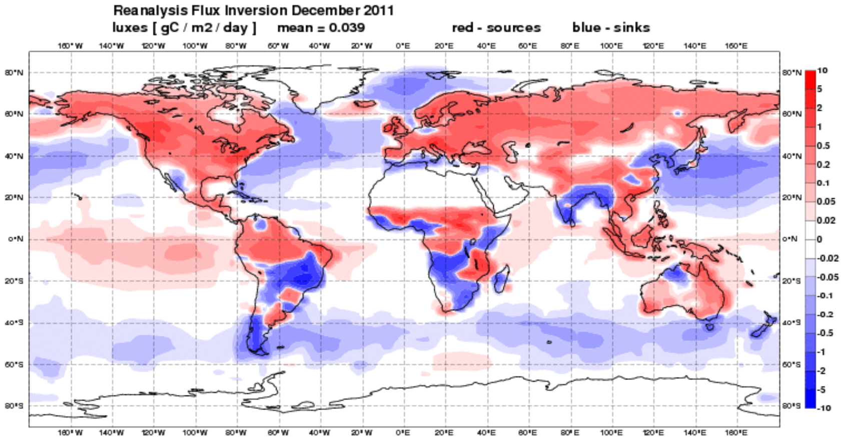
NWP 4D-Var is mostly defined as an initial value problem. Only initial conditions are changed and model error is relatively small.

1. Examples of emissions

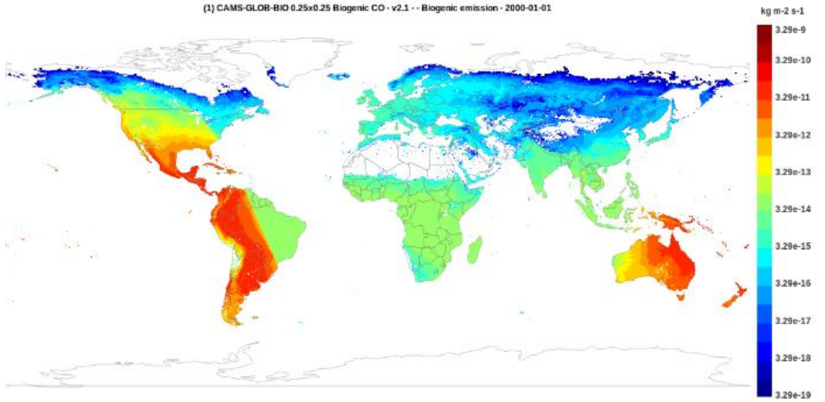
TNO European anthropogenic NOx emissions



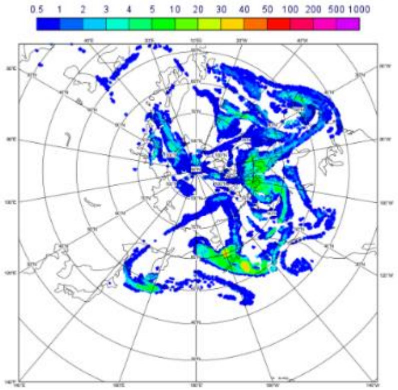
CO_2 fluxes



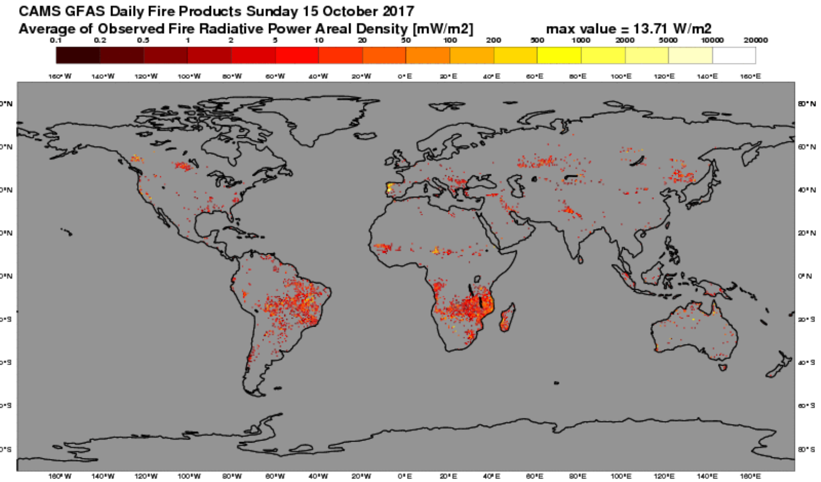
CAMS_GLOB biogenic CO emissions



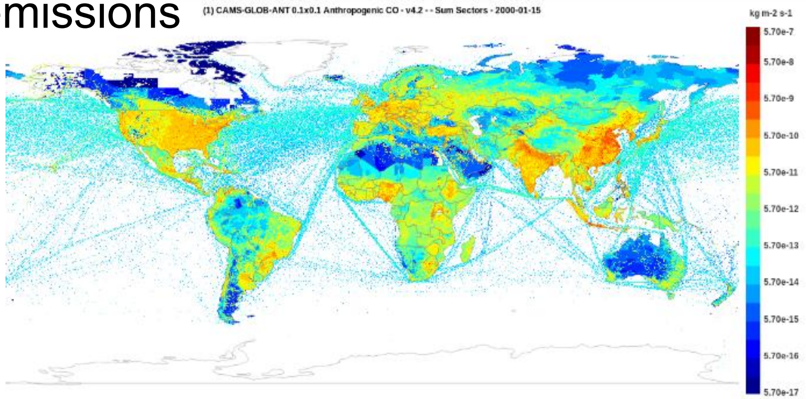
Volcanic SO_2



Biomass burning, 15 October 2017

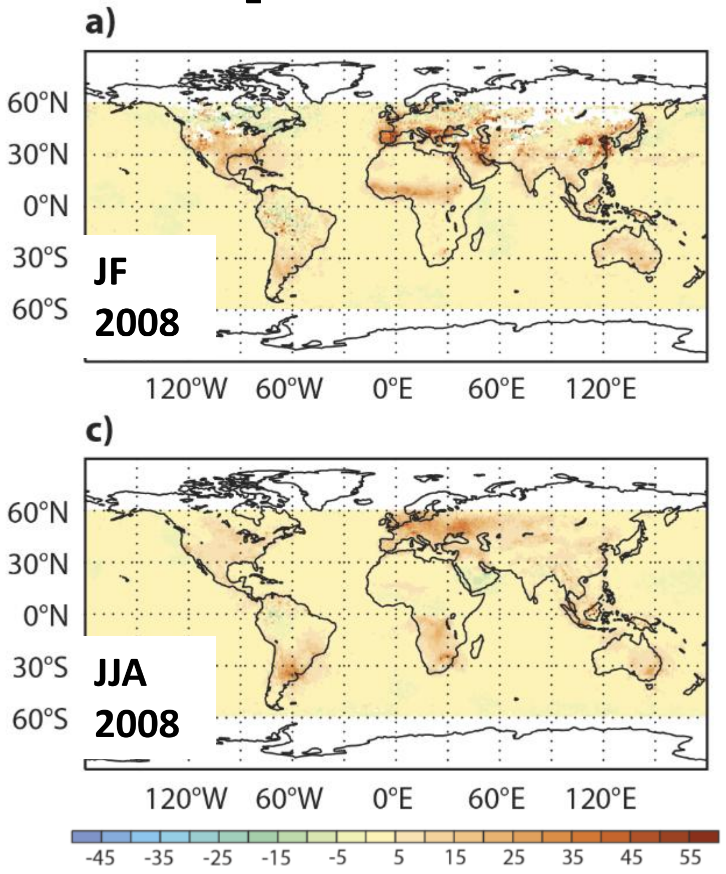


CAMS_GLOB anthropogenic emissions

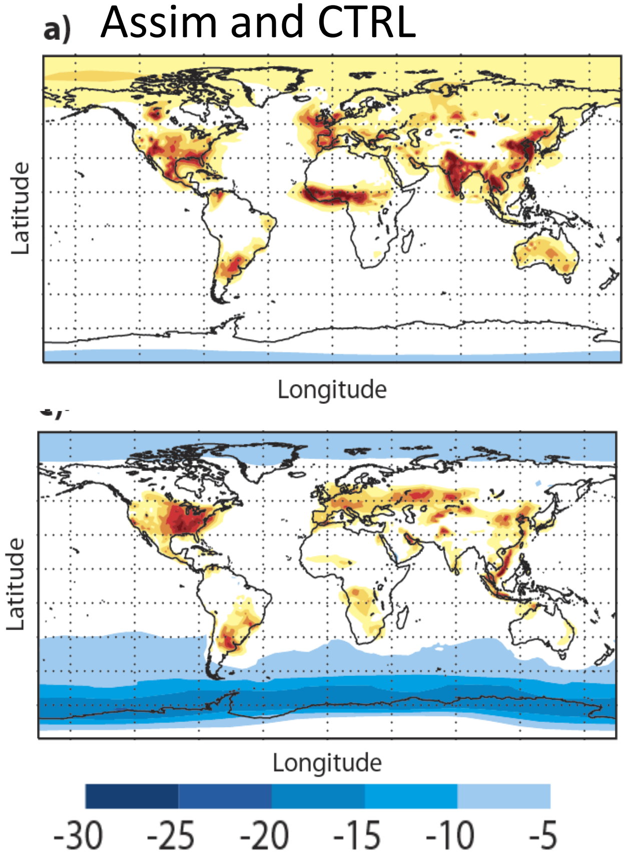


1. Short-lived memory of NO_2 assimilation

OMI NO_2 analysis increment [%]



Differences between Assim and CTRL



- Large positive increments from OMI NO_2 assim
- Large differences between analyses of ASSIM and CTRL

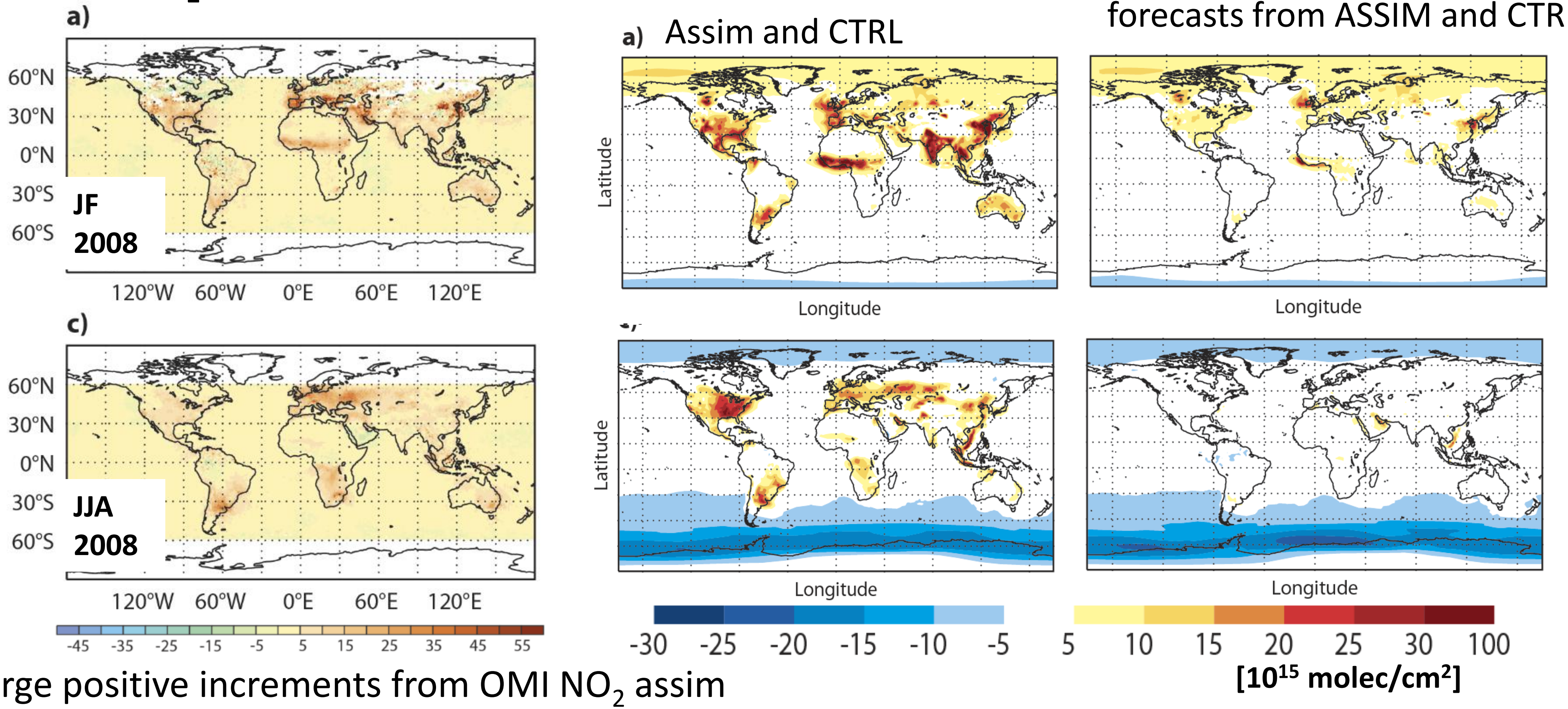
Inness et al. (2015, ACP)

1. Short-lived memory of NO_2 assimilation

OMI NO_2 analysis increment [%]

Differences between Assim and CTRL

Difference between 12h forecasts from ASSIM and CTRL



- Large positive increments from OMI NO_2 assim
- Large differences between analyses of ASSIM and CTRL
- Impact is lost during subsequent 12h forecast
- Constraining emissions (in addition of IC) would give a better initial state and persistence of forecast improvements throughout the DA window

Inness et al. (2015, ACP)

1. Joint state/emissions 4D-var inversion system

$$J(x,p) = \overbrace{(x - x_b)^T B^{-1}(x - x_b)}^{J_b\text{: background constraint for x}} + \overbrace{(p - p_b)^T {B_p}^{-1}(p - p_b)}^{J_p\text{: constraint for emission scaling factors}}$$

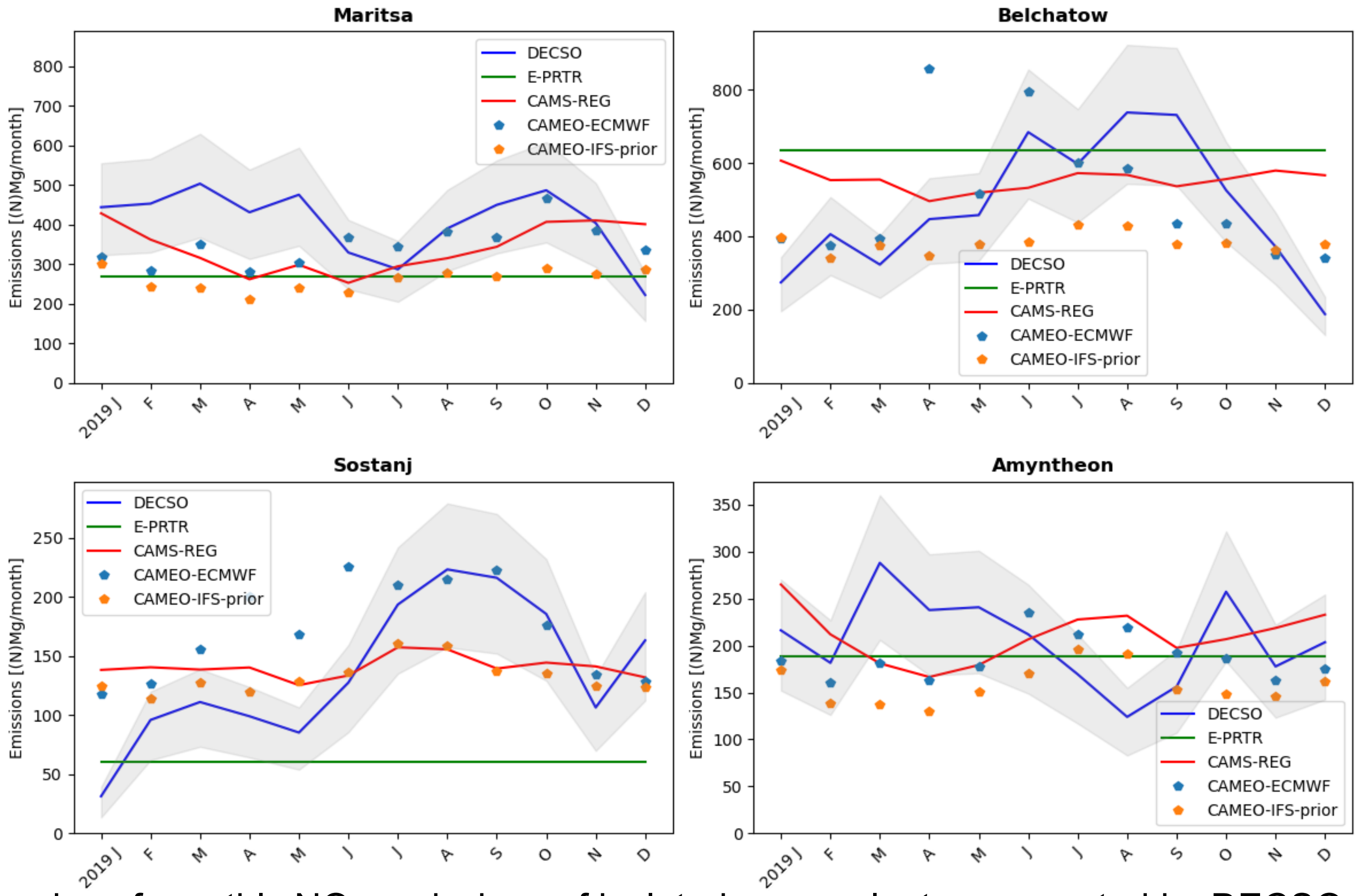
State control vector

Parameter (e.g. scaling factors)

$$+ \underbrace{\sum_{i=0}^{n}(y_i - H_i[x_i, p])^T R_i^{-1}(y_i - H_i[x_i, p])}_{J_o\text{: observation}}$$

- Joint optimisation of emissions and initial conditions
- Optimized emissions for e.g., CO_2, CH_4, CO, NO & NO_2
- TL/AD of simplified chemistry: link between NO emissions and NO_2 observations
- 2D scaling factors p applied to emission fields
- Prior error definition:
  - Global constant or 2D map of standard error
  - Spatial correlation length scale (via B_p)
  - NO/CO_2 emission error correlation in B_p -> NO_2 obs can constrain CO_2 emissions

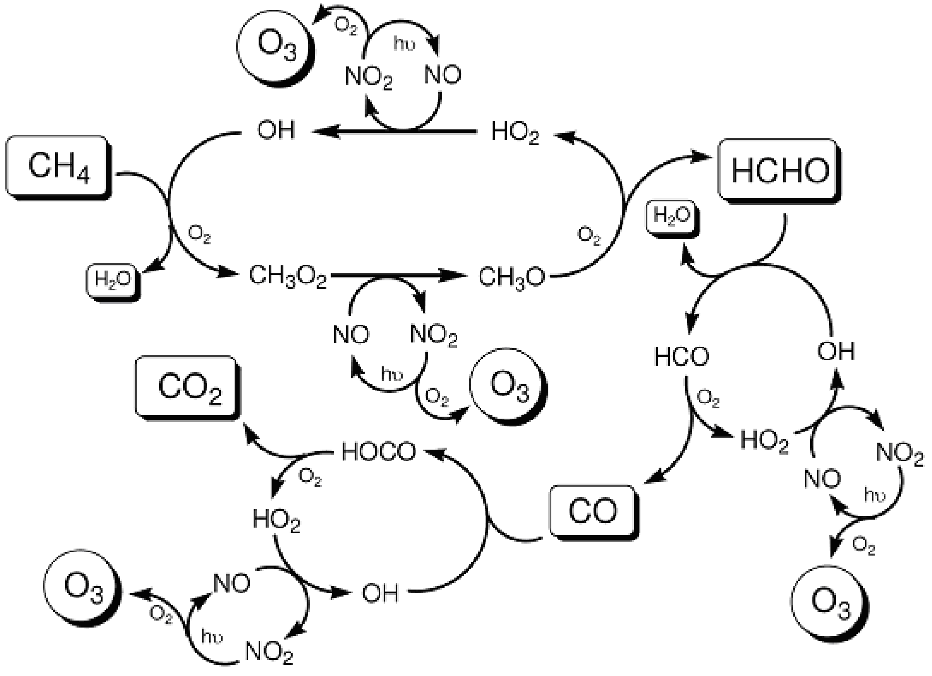
1. No_x inversion results: power plants

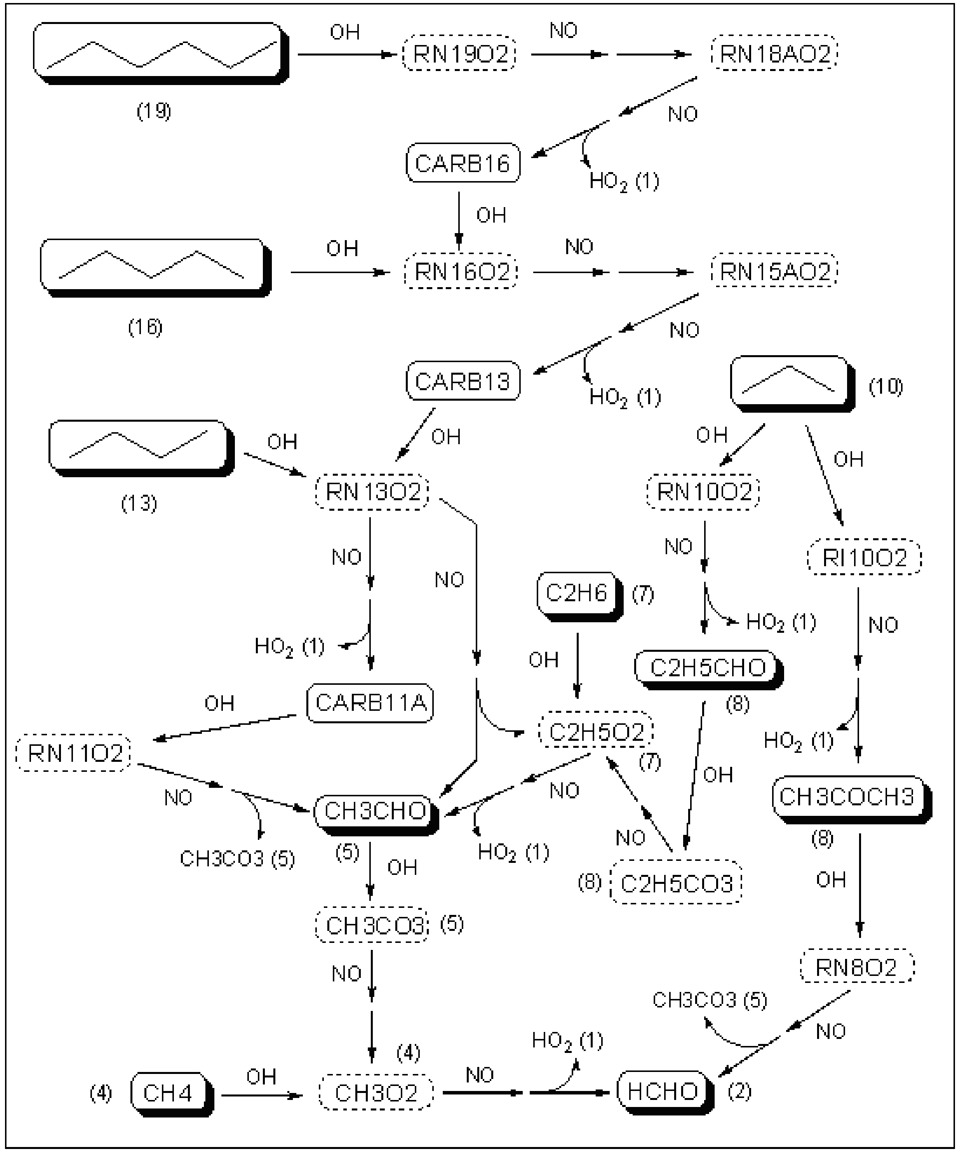


- <u>Power plants</u>: IFS posterior generally in better agreement with independent higher resolution top-down inversion than prior emissions.

Time series of monthly NOx emissions of isolated power plants as reported by DECSO (blue line), E-PRTR (green line), CAMS-REG (red line), CAMEO-ECMWF (blue dots) and CAMEO-ECMWF prior (orange dots). The grey shadow regions show the estimated uncertainty of the DECSO emissions.

2. Dealing with many (reactive) atmospheric species

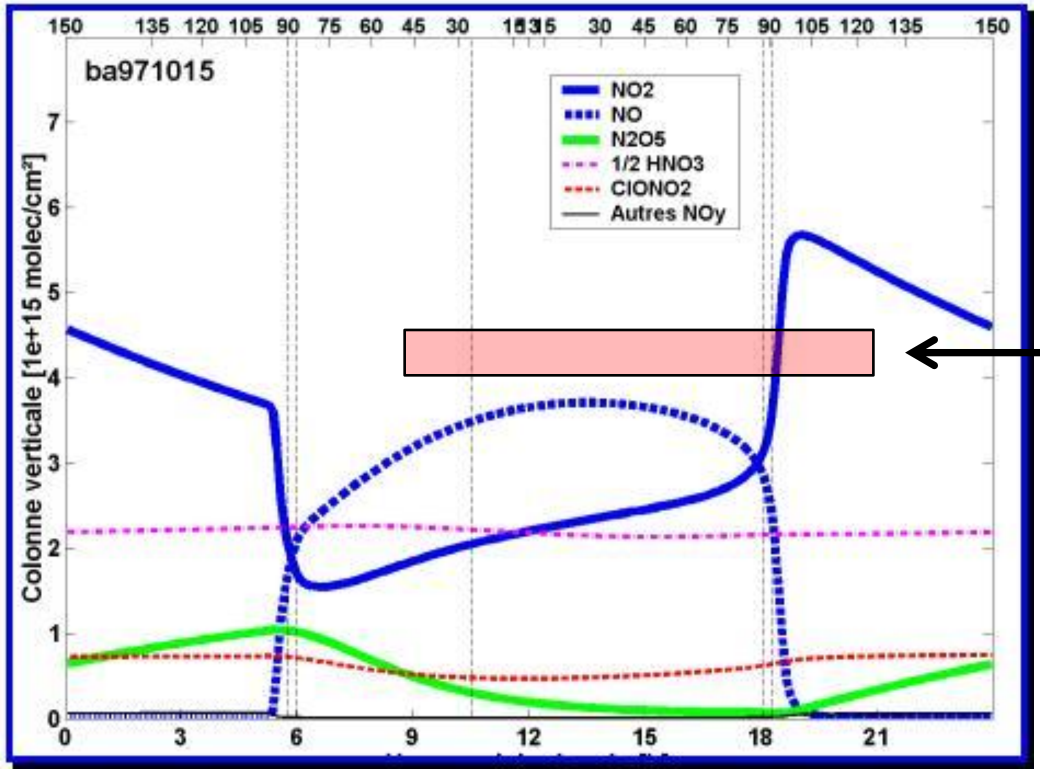




Complexity can go very far… with master mechanisms of about 10000 variables

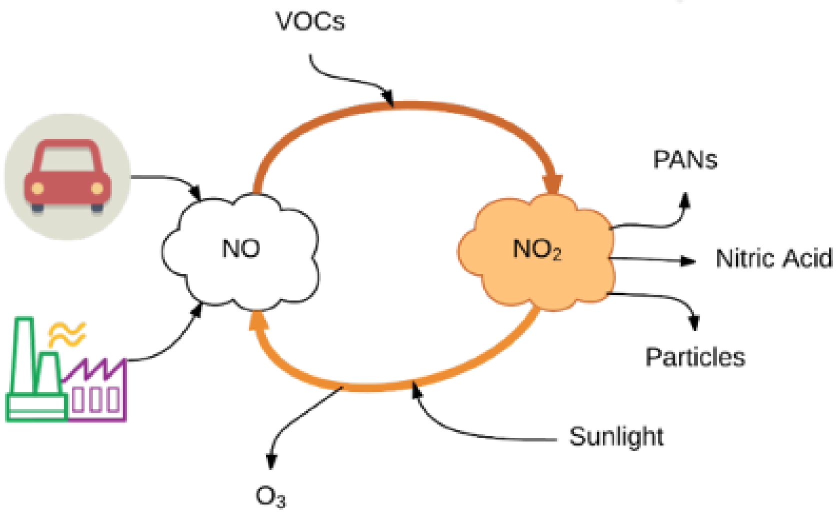
Usually, it is costly to model and simplifications are mandatory to run an operational forecasting system with only around 100 variables.

2. Example: assimilating NO_2 satellite observations



Credits: J-C Lambert (BIRA)

12-hour
4D-Var
window



Rapid chemical conversion within the 12-hour 4D-Var window means we cannot link an NO_2 observation at the end of the window correctly to the initial state without a full chemical adjoint.

2. Include simple chemistry in TL/AD

Photochemical equilibrium:

- $NO + O_3 \rightarrow NO_2$
- $NO_2 + h\nu \rightarrow NO + O_3$

Loss term for NOx:

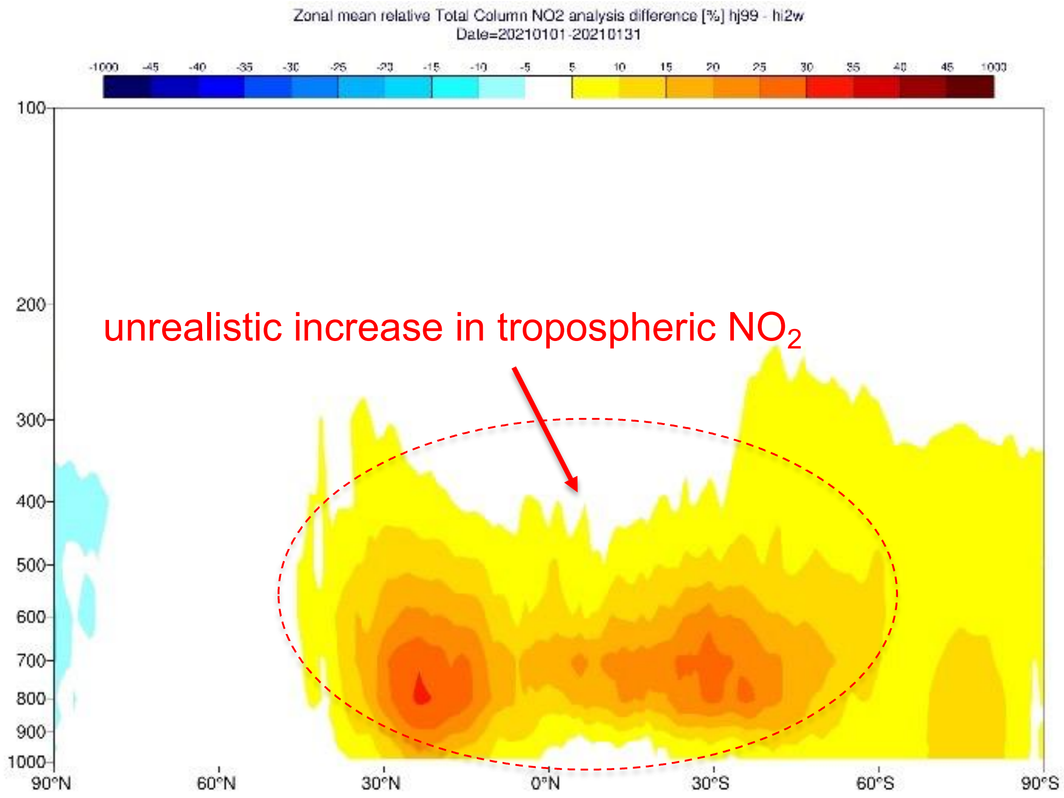
- $NO_2 + OH \rightarrow HNO_3$

> - Uses non-linear O_3, NO, NO_2, OH trajectory as linearization state.
> - Only NO_2, NO increments are propagated
> - Assume instantaneous equilibrium (no sub-time stepping).

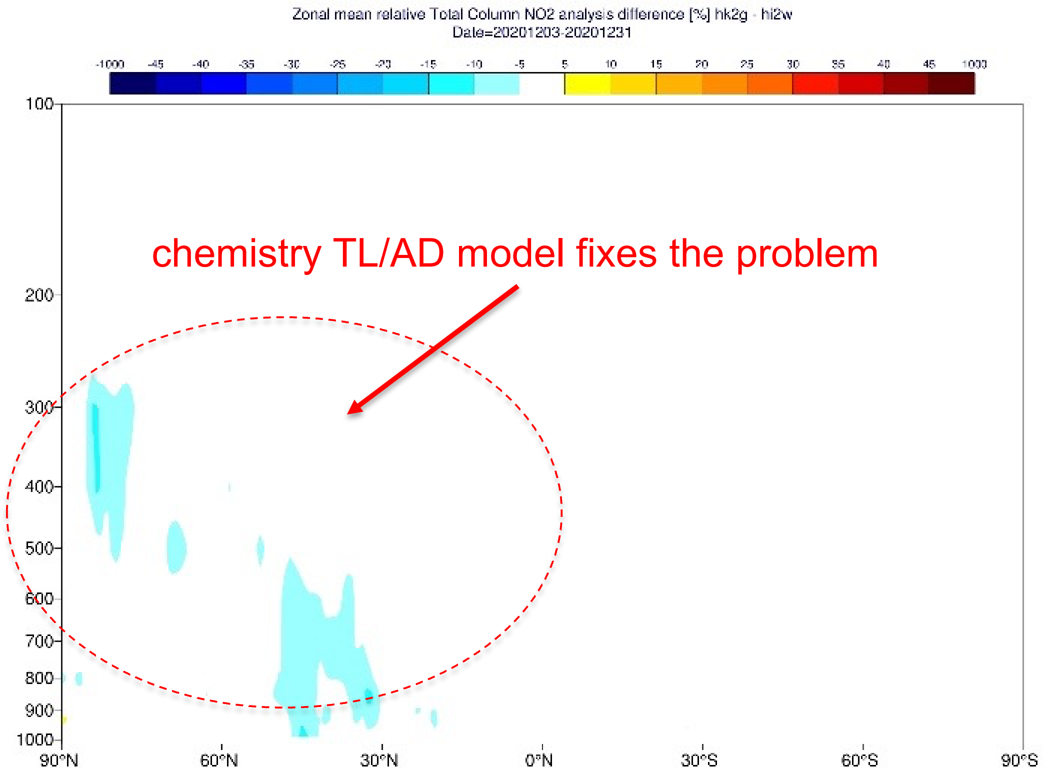
2. Simplified chemistry TL/AD

Impact of TROPOMI NO_2 assimilation

No chem - CTRL



Simplified chem - CTRL



3-31/12/2020

Relative zonal mean differences [%]

3. Mismatch between modelled and observed variables

$$J(x) = (x \quad \cdots \quad) + \sum_{i=0}^{n} (y_i - H_i[x_i])^T R_i^{-1} (y_i - H_i[x_i])$$

Control variables

NWP

vorticity
divergence
temperature
surface pressure (logarithm)
specific humidity

Atmospheric Composition

ozone
carbon monoxide
nitrogen dioxide
formaldehyde
sulphur dioxide

carbon dioxide
methane

aerosol mixing ratio

Only a small subset of all chemical species are observed and therefore included in the control vector. This means the full chemical system is very under-constrained.

3. Mismatch between modelled and observed variables

Control variables

NWP

vorticity
divergence
temperature
surface pressure (logarithm)
specific humidity

Atmospheric Composition

Total column and profile observations

ozone
carbon monoxide
nitrogen dioxide
formaldehyde
sulphur dioxide

Total column observations

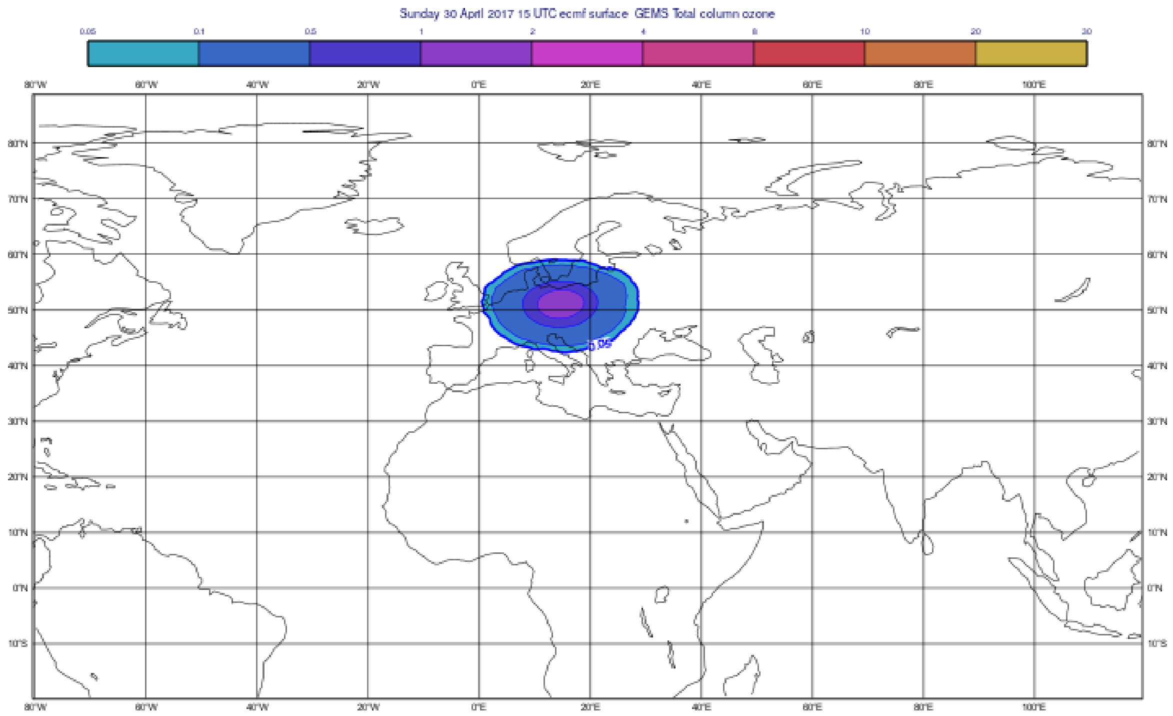
carbon dioxide
methane

aerosol mixing ratio

$$J(x) = (x \qquad) + \sum_{i=0}^{n} (y_i - H_i[x_i])^T R_i^{-1} (y_i - H_i[x_i])$$

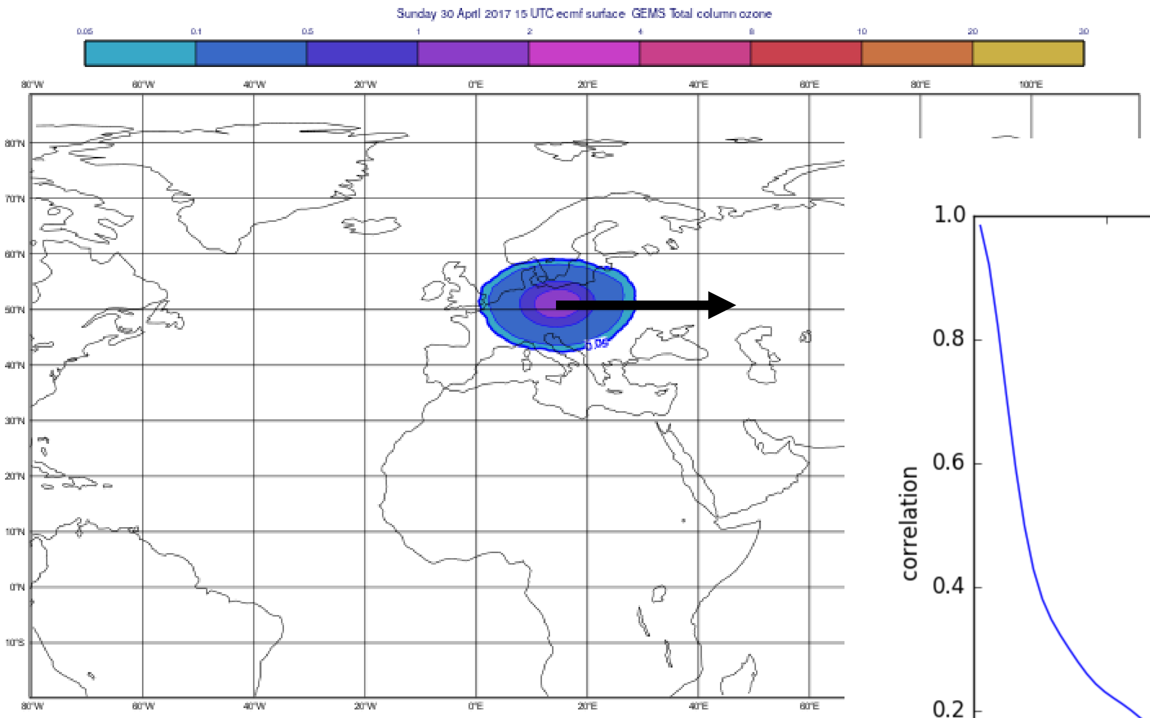
Even for those species that are observed, it is often only total column data that is available.

3. Increment from a single total column ozone observation



Increment created by a single ozone observation of 375 DU, 10 DU higher than background

3. Increment from a single total column ozone observation



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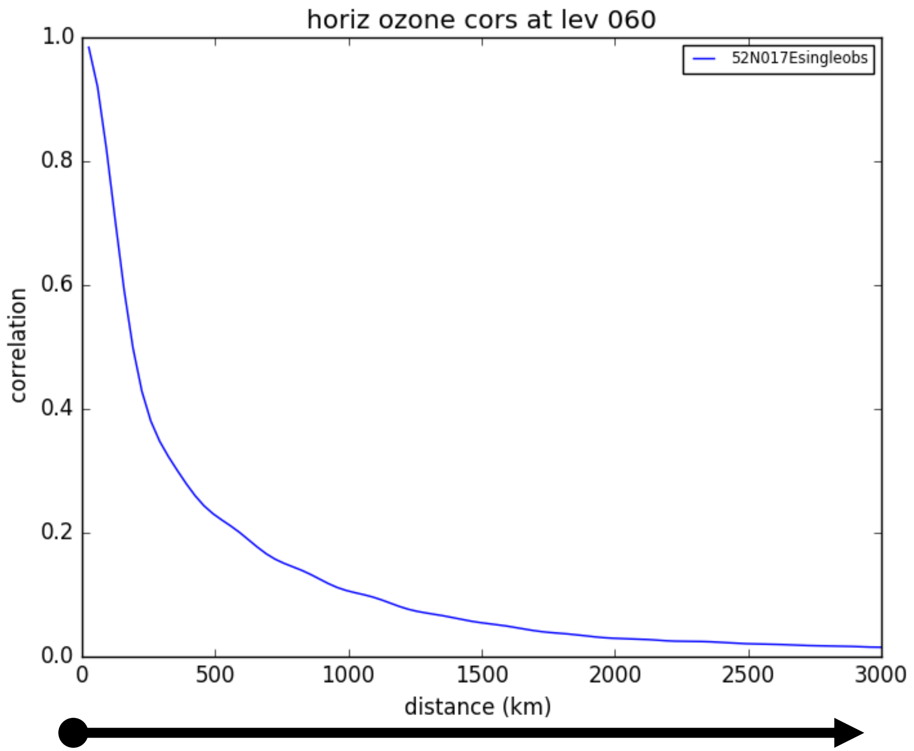

Horizontal correlation from the B-matrix that spreads the information from the single observation in the horizontal

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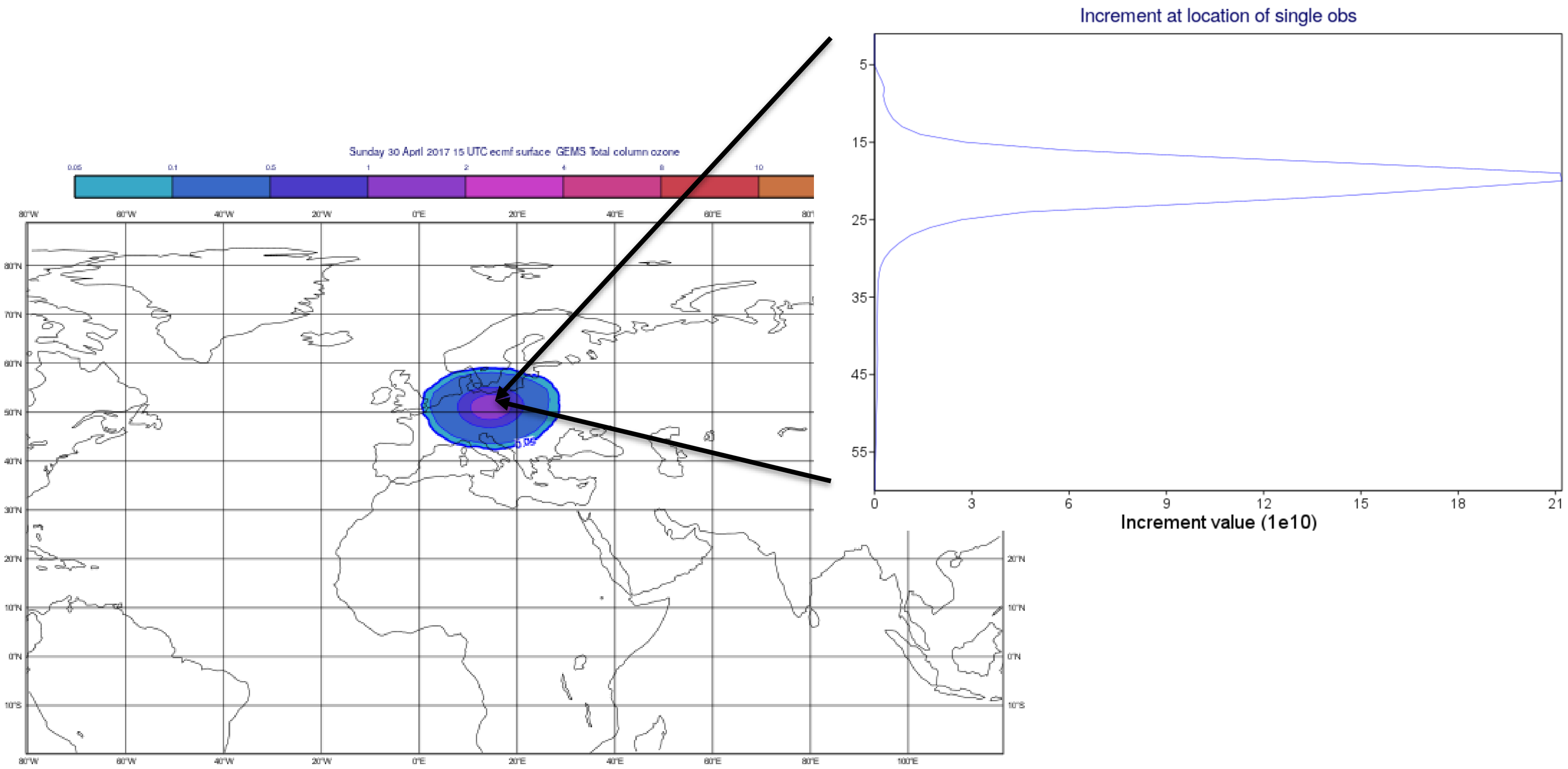

Vertical profile of the increment at the observation location

Increment created by a single ozone observation of 375 DU, 10 DU higher than background

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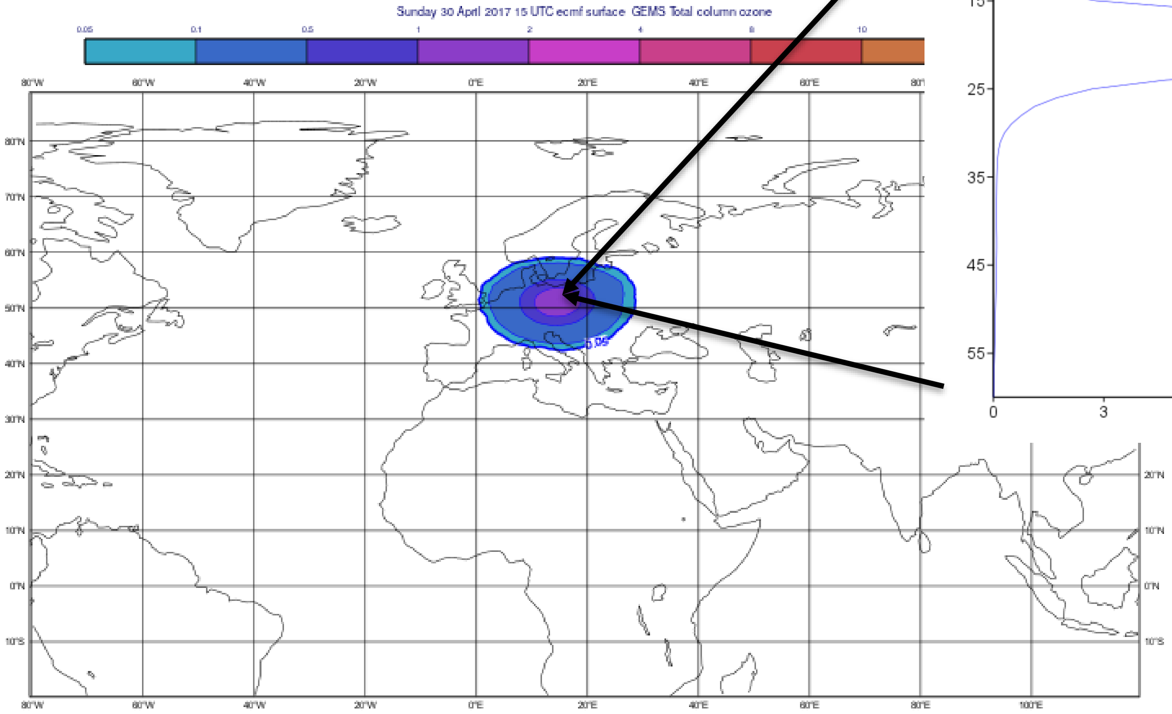
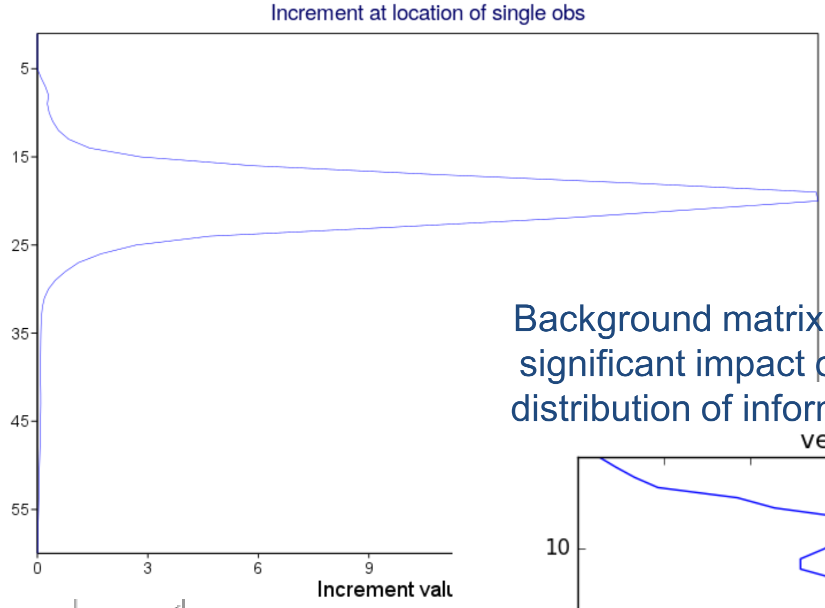
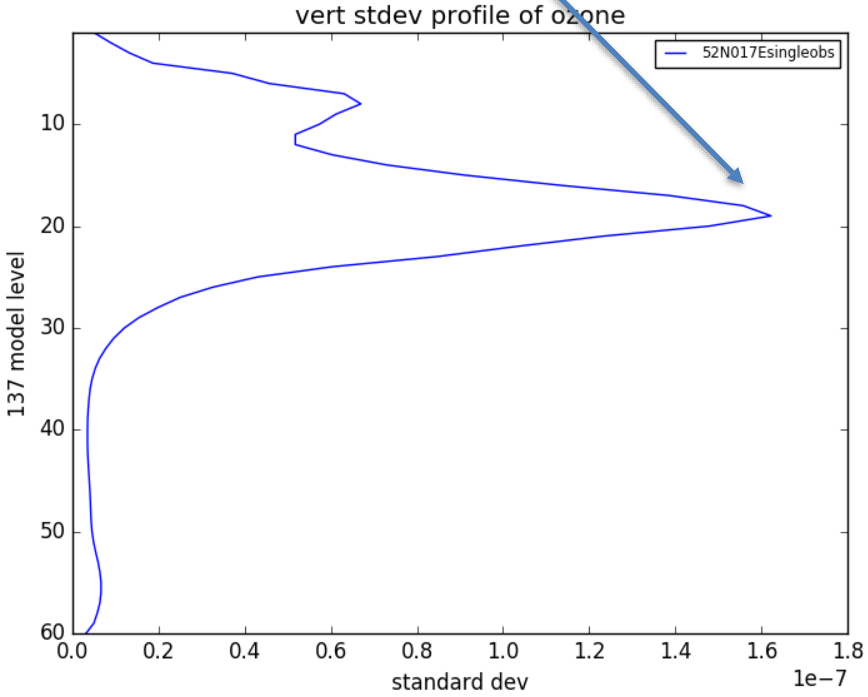




Vertical profile of the increment at the observation location

Background matrix has a significant impact on the distribution of information

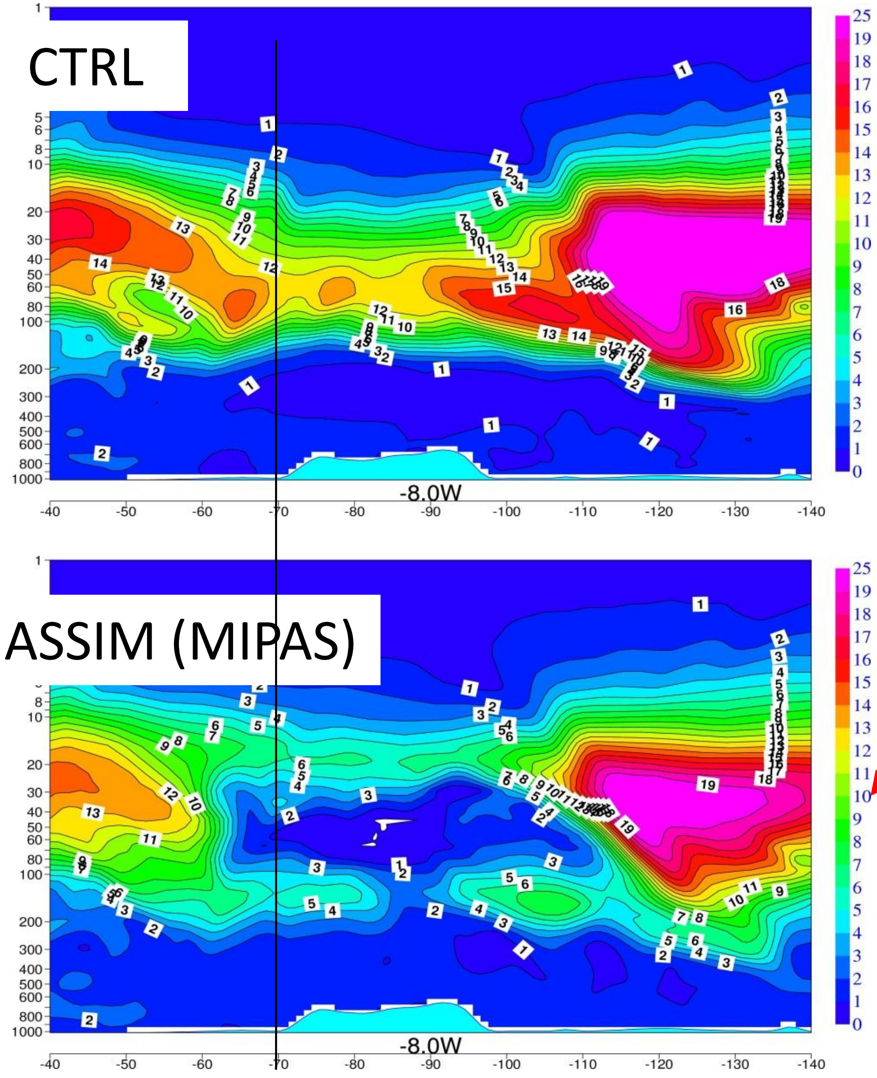


Increment created by a single ozone observation of 375 DU, 10 DU higher than background

Standard deviation from the background matrix at the observation location

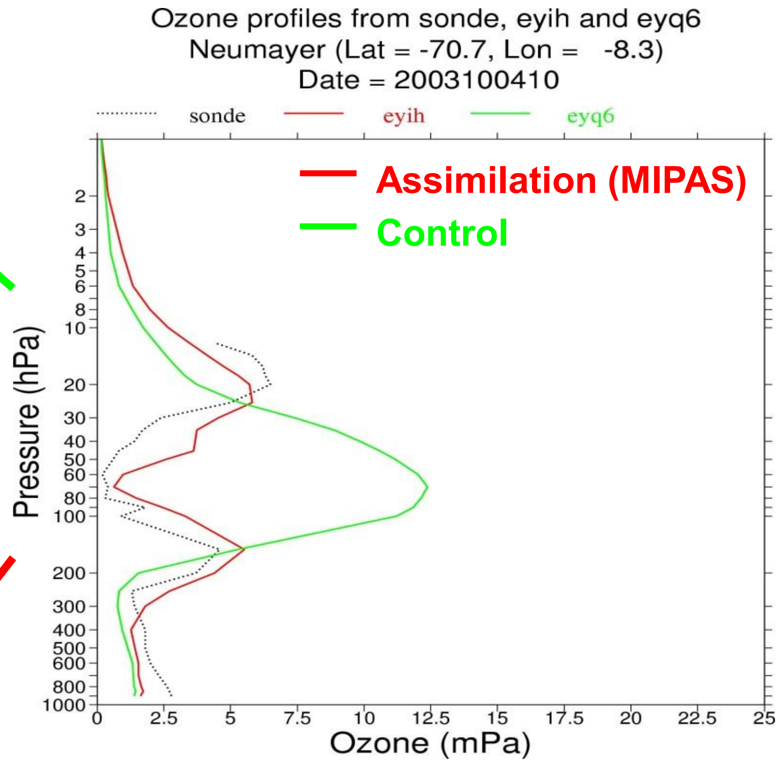
Formulation of the B-matrix is very important for AC

3. Benefit of profile information – B matrix is not enough!



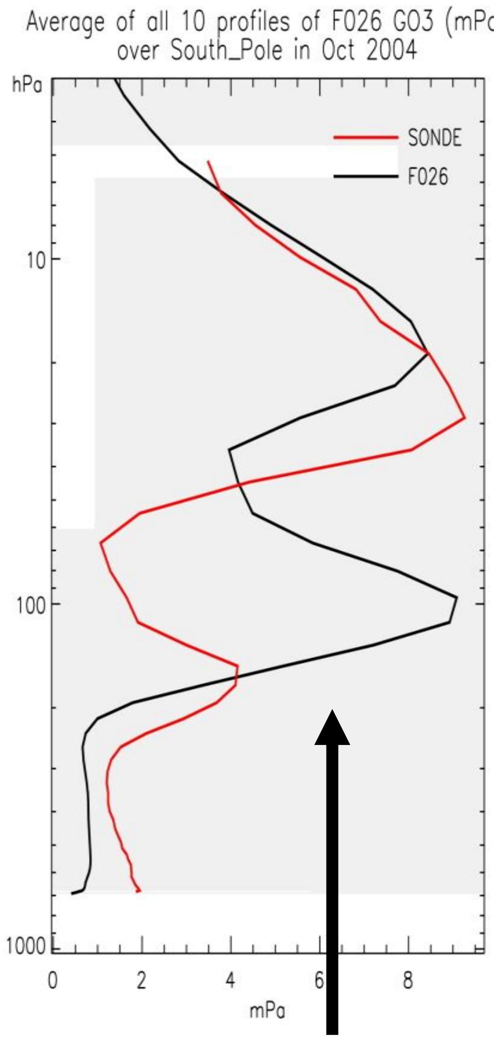
70S

Ozone hole in CAMS reanalysis: Cross section along 8E over South Pole, 4 Oct 2003



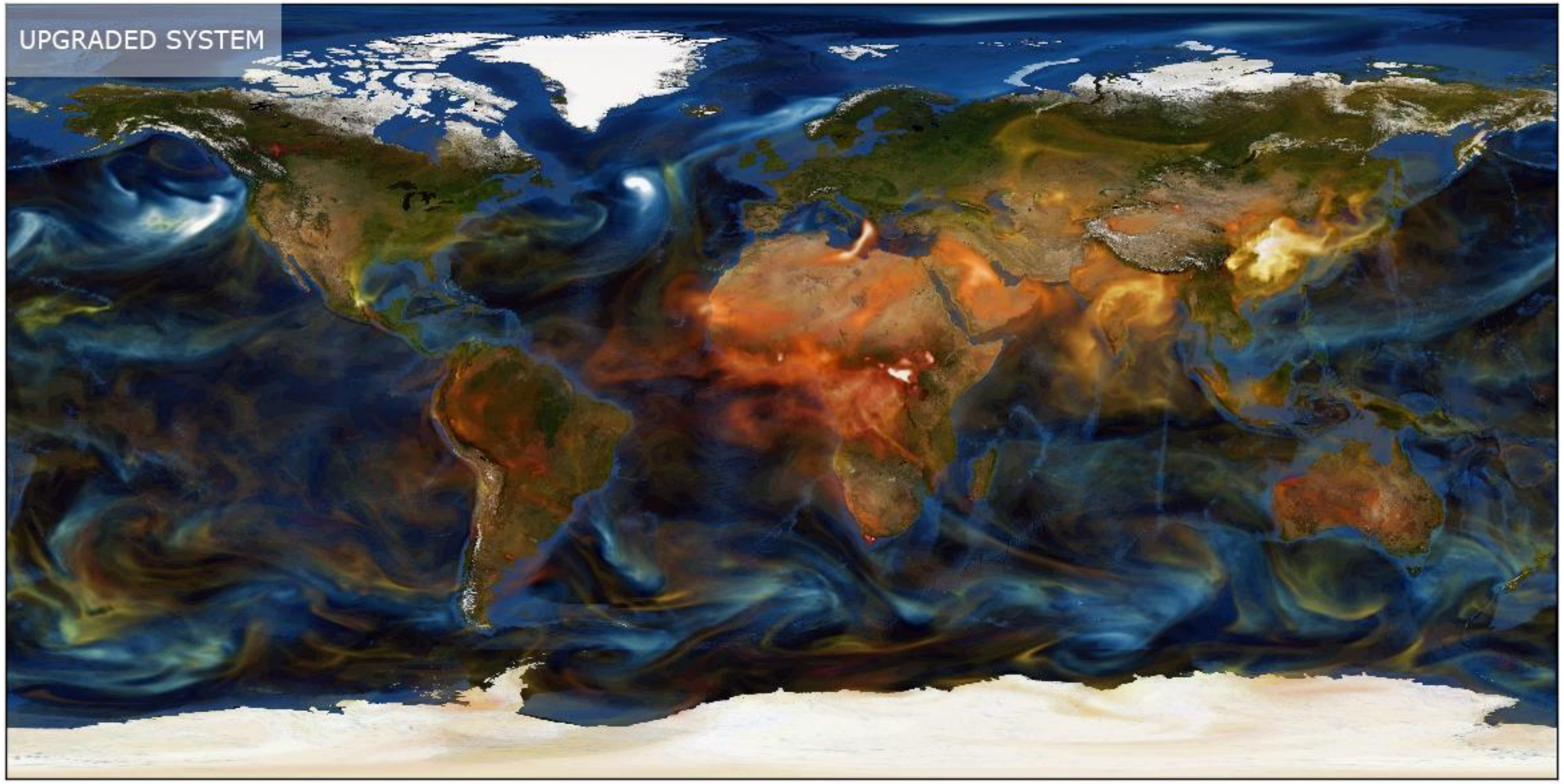
Assimilation **with profile data**

Oct 2004



Assimilation **with total column data**

3. Aerosol – prime example of ill-observed system



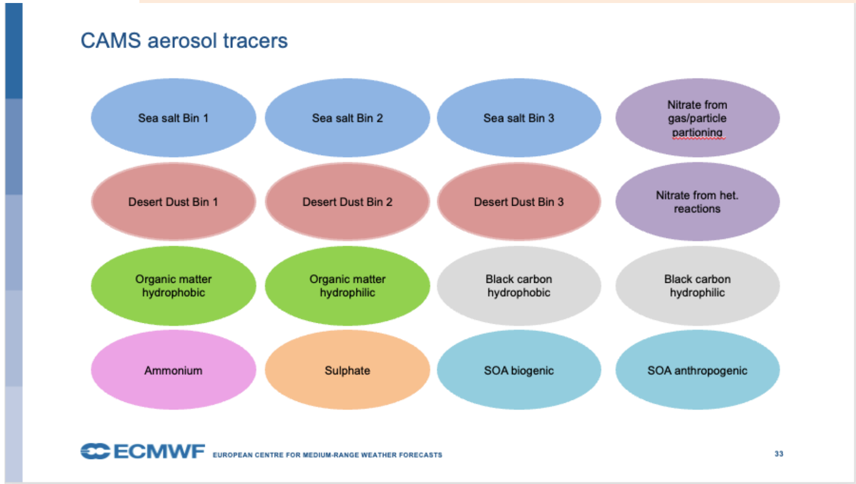
12-hour CAMS forecasts of dust (orange), sea salt (blue), biomass burning (red) and sulphate aerosols (yellow), 12 UTC on 18 January 2017

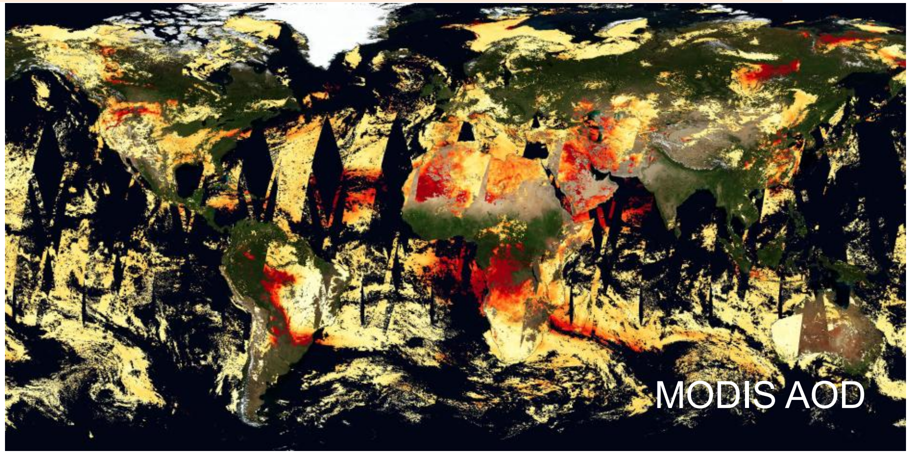
CAMS aerosol tracers

- Sea salt Bin 1
- Sea salt Bin 2
- Sea salt Bin 3
- Nitrate from gas/particle partioning
- Desert Dust Bin 1
- Desert Dust Bin 2
- Desert Dust Bin 3
- Nitrate from het. reactions
- Organic matter hydrophobic
- Organic matter hydrophilic
- Black carbon hydrophobic
- Black carbon hydrophilic
- Ammonium
- Sulphate
- SOA biogenic
- SOA anthropogenic

AOD observations

- Model fields are aerosol mixing ratios of 16 tracers
- Assimilated data are total AOD at 550 nm (e.g. from MODIS, VIIRS, PMAp)
- We need to transform aerosol mixing ratios into total AOD





Credit: Nasa Worldview

Forward AOD observation operator steps:

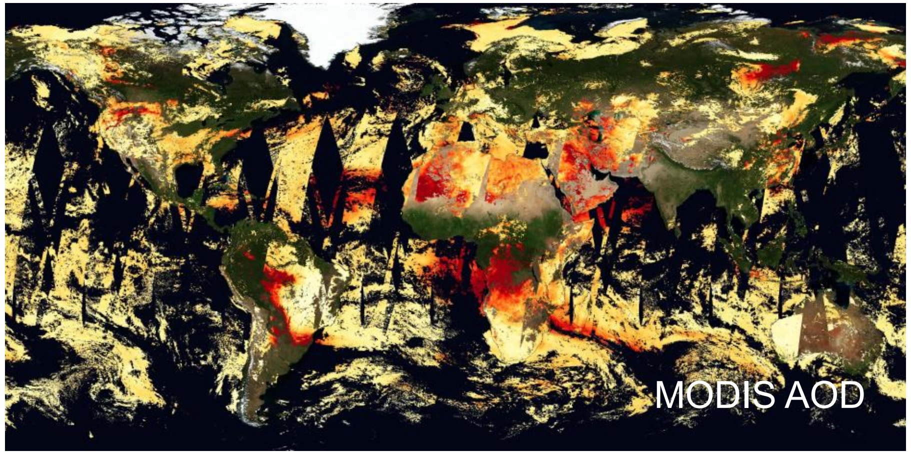
Control variable is ***total aerosol mixing ratio***

1. Interpolate aerosol mass mixing ratios to obs location & time
2. Calculate model RH: it has impact on the optical properties of hygroscopic aerosol
3. Get mass extinction coef at waveleghth (e.g. 550 nm) from a look-up table
4. Multiply (3) * (1) to get single-species AODs
5. Total AOD is sum of single-species AOD

$$\tau_\lambda = \sum_{i=1}^{N} \int_{p_{surf}}^{0} \alpha_{ei}(\lambda, RH(p)) r_i(p) \frac{dp}{g},$$

Straight forward

Adjoint AOD observation operator



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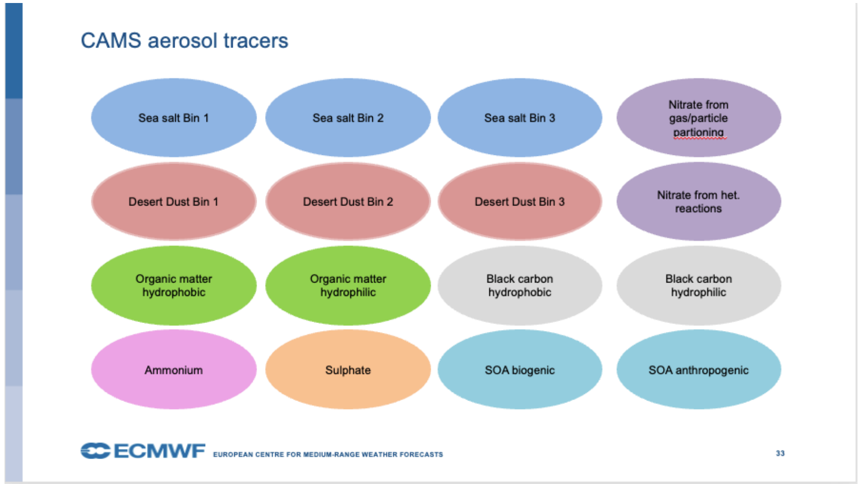


Adjoint AOD observation operator steps:

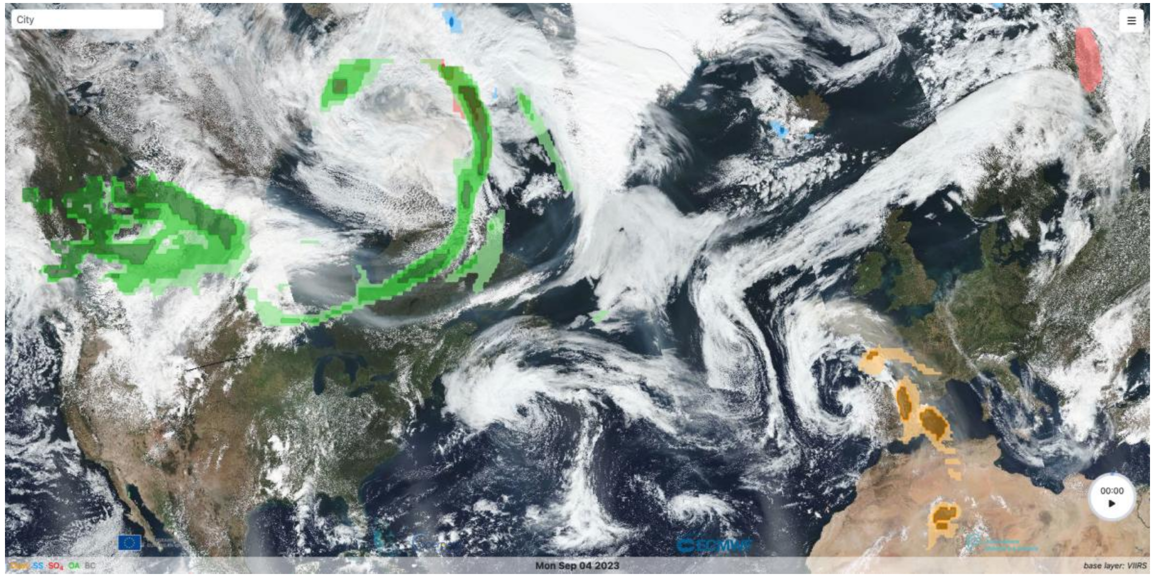
- AOD analysis increments transferred to total aerosol mixing ratio
- Analysis increments are repartitioned into the 16 species according to their fractional contribution to the total aerosol mixing ratio of the background forecast
- Largest contribution for dominant aerosol species
- Can not ‘create’ a species if not present in background forecast
- The repartitioning of the total aerosol mixing ratio increment into the different bins can lead to problems with the aerosol speciation

Not well constrained

Examples of CAMS aerosol species

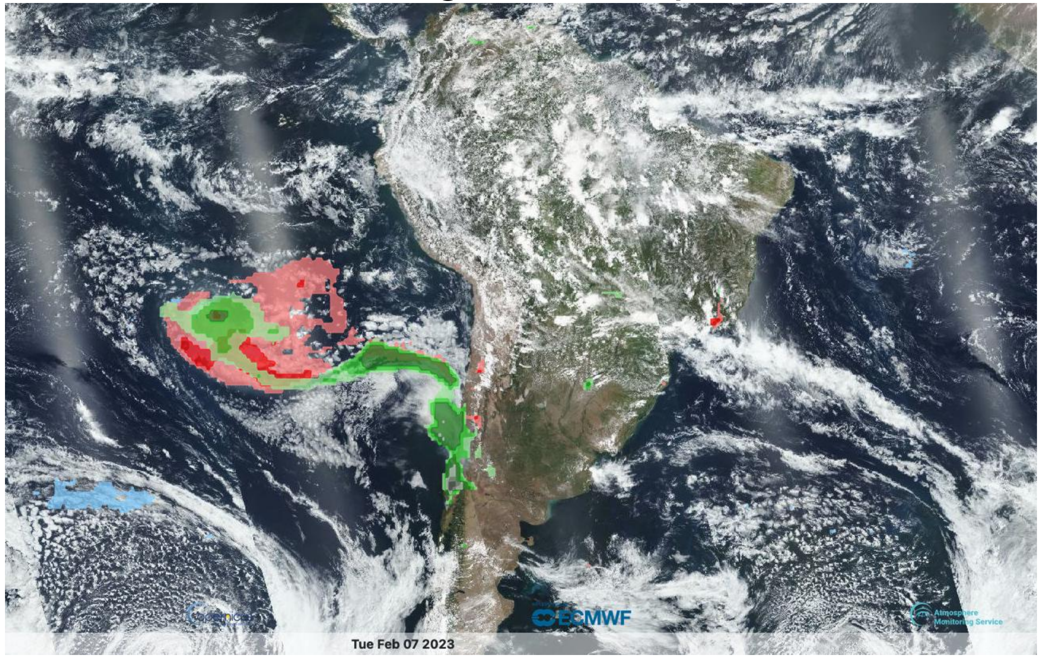
CAMS aerosol alerts:
https://aerosol-alerts.atmosphere.copernicus.eu/

Good example



Organic matter, desert dust, sea salt, sulphate

Not so good example



Part of fire plume is attributed to sulphate which is the dominant species in background forecast

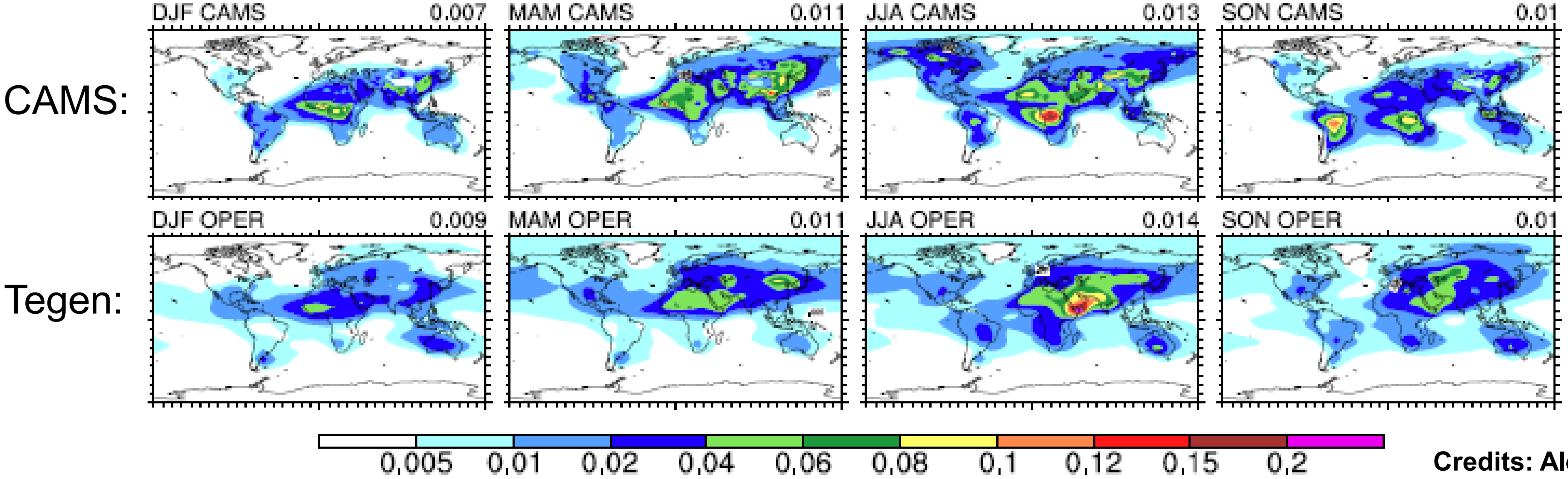
Area being investigated:

- Use of single species observations (IASI thermal infrared radiances can pick up coarse dust particles)
- New instruments, such as 3MI, can pick up more information on the aerosols, e.g. Size information or whether the aerosol is absorbing

Potential Benefit for NWP

Benefit of AC for NWP: Updated climatology in the radiation scheme

Climatological AOD 550nm distribution CAMS vs Tegen et al 1997

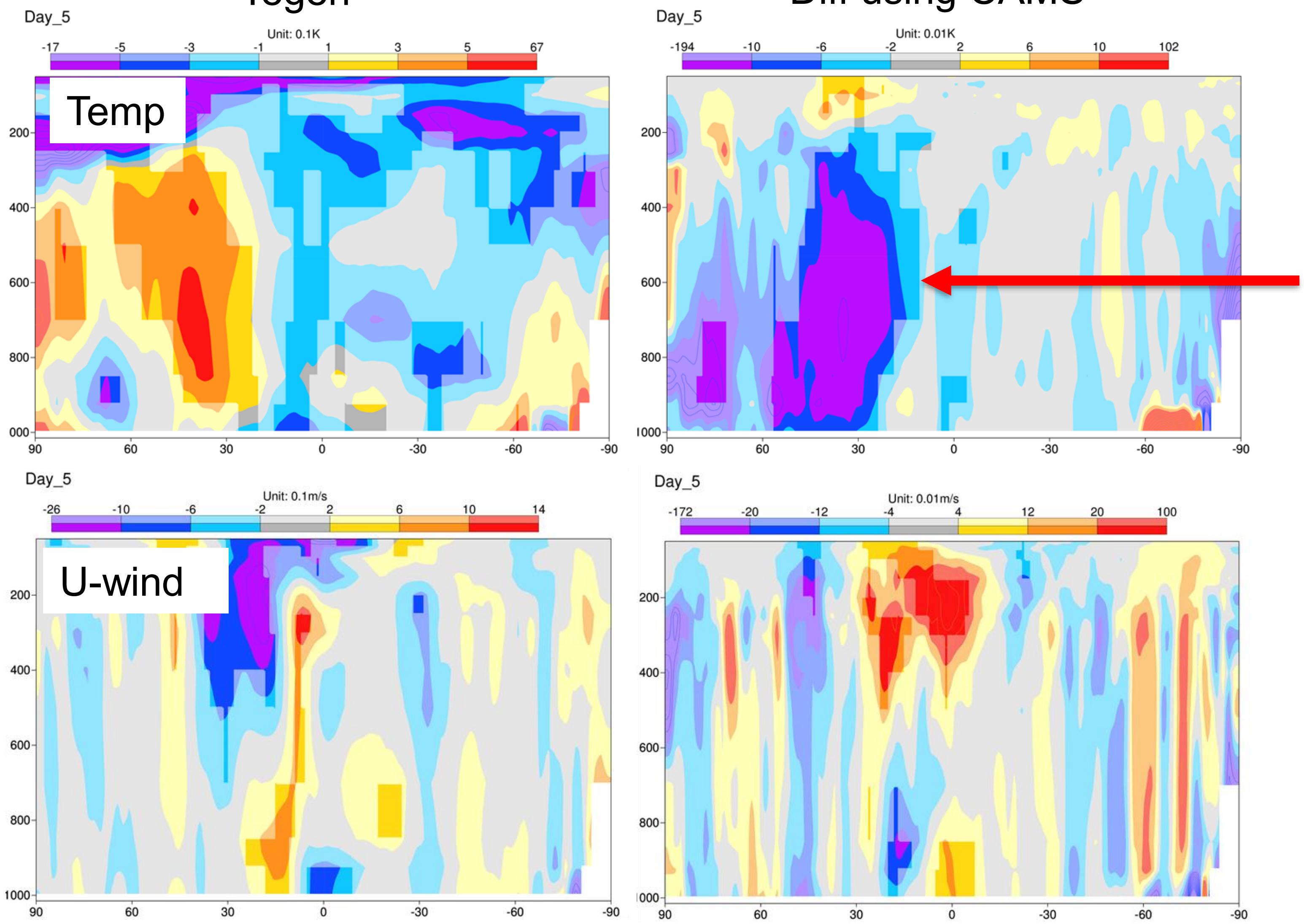


Credits: Alessio Bozzo

- CAMS interim reanalysis (2003-2018): sources of biomass burning from GFAS, sulphate aerosol precursor from EDGAR 4.1, prognostic for sea salt and dust, revised dust model
- Optical properties recomputed for RRTM spectral bands and for each aerosol type/size bin. Mass mixing ratio as input to radiation
- Vertical distribution following an exponential decay with scale height derived from the CAMS model for each aerosol type. Monthly varying for dust.

Improvements to NWP forecast errors

Tegen | Diff using CAMS



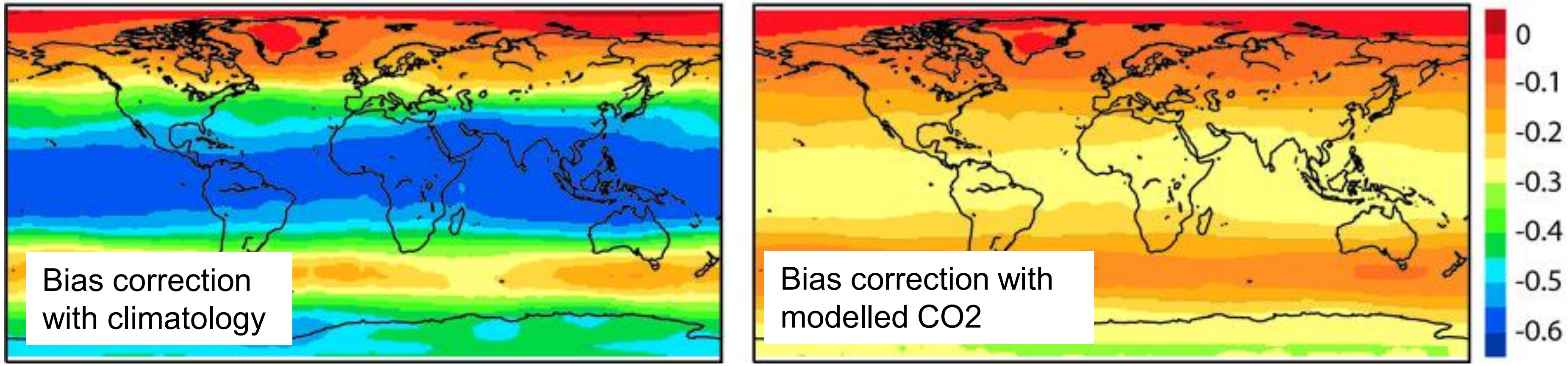
June-July
Model FC error d+5

June-July
Change in FC error d+5

- Change in mass distribution and optical properties -> reduction in SW absorption -> reduction in temperature (positive)
- This is of the order of 0.1K for a bias of the order of 0.3K – it explains at least ~30% of the temperature error.
- Similar for winds at upper levels

Benefit of AC for NWP: Variable CO2 in radiance assimilation

Reduced AIRS and IASI Bias Correction



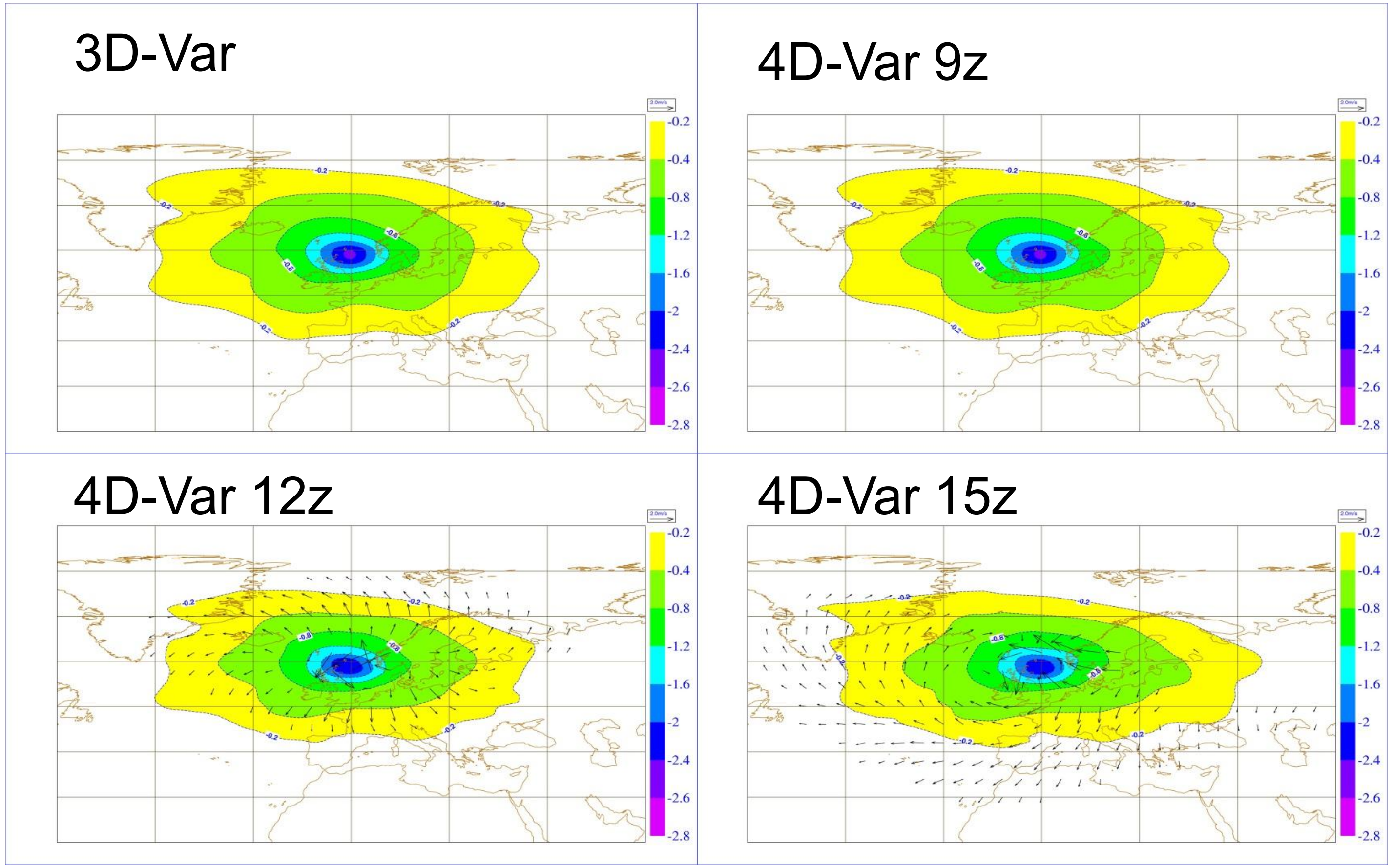
Mean bias correction (K) for August 2009 for AIRS channel 175 (699.7 cm^{-1}; maximum temperature sensitivity at ~ 200 hPa)

Engelen and Bauer, QJRMS, 2011

- Using modelled CO_2 in AIRS/IASI radiance assimilation leads to significant reduction in needed bias correction.
- Small positive effect on T analysis and neutral scores/ small positive impact at 200 hPa T in Tropics
- Stratospheric T in variable CO2 exp more consistent with AMSU-A
- It would be beneficial to replace the fixed value by more realistic values

Benefit of AC for NWP: Wind information from tracers

- Prospect to extract wind information from long lived tracers in stratosphere and upper troposphere, e.g. O_3, H_2O, N_2O.
- Potential to extract wind info indirectly through TL and AD of tracer advection
- Could compliment existing wind observations and help in areas where there is a lack of adequate global wind profile data



Level 20 ≈ 30 hPa

Observation at T0: 4D-Var = 3D-Var

Observation at T3: wind increments

Observation at T6: wind increments

6h assimilation window

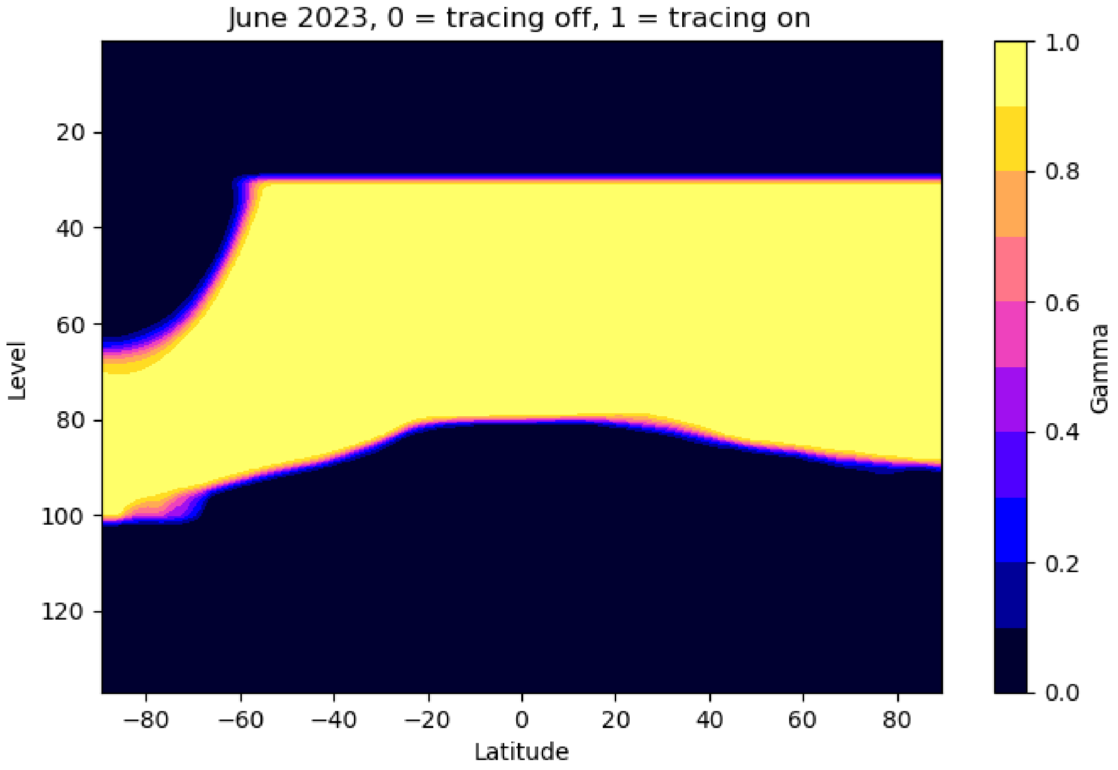
Benefit of AC for NWP: To be included in the next model upgrade (CY50r1)

- Tracing turned off:
    - In the mid- and lower-troposphere
    - In the 4D-Var sponge layer (above 10 hPa)
    - In the areas with T<195 K, where less predictable heterogeneous chemistry is an important contributor to $\partial r(O_3)/\partial t$ in the nonlinear model

- Different γ for each month based on ERA5 climatology

- Fully flow-dependent γ based on latest background

$$\gamma(x, y, \eta, t)$$



Parameter γ controls the “level” of tracer-wind coupling in the assimilation

Zaplotnik, Ž., Žagar, N. & Semane, N.(2023) Flow-dependent wind extraction in strong-constraint 4D-Var. Quarterly Journal of the Royal Meteorological Society, 149(755, 2107–2124

Potential benefit for NWP

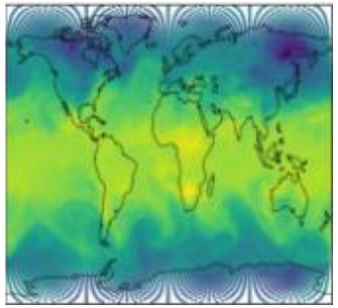
- Interactive aerosols: Feedback on dynamics via radiation scheme: First Tegen AER climatology used in radiation scheme, CAMS interim climatology from CY43R3 onwards
- Use of O3 (& other fields) in the radiation scheme: MACC climatologies used
- RTTOV observation operator: Use of O3, CO2 analysis fields to improve the use of radiances sensitive to O3, CO2: model O3 is used, but climatologies used for other tracers (e.g. fixed CO2 value)
- Dynamical coupling with wind/T through TL and AD: turned on under specific conditions

Machine Learning for Atmospheric Composition

From AIFS to AIFS-Compo

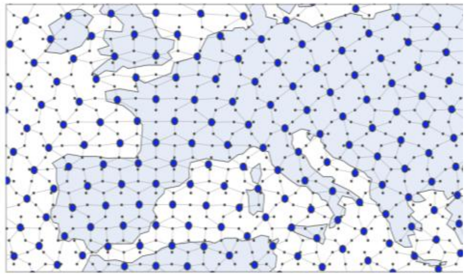
Machine Learning for AC forecasting is in principle no different from machine learning for NWP AI forecasts

Input
Atmospheric state+AC variables:
X(t), X(t-3h)

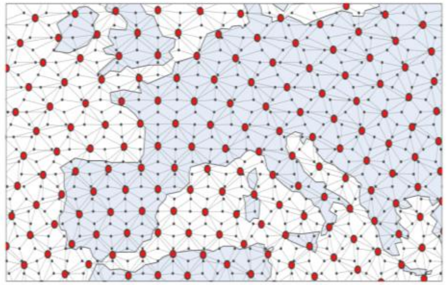


AIFS-Compo MODEL

encoder → processor → decoder

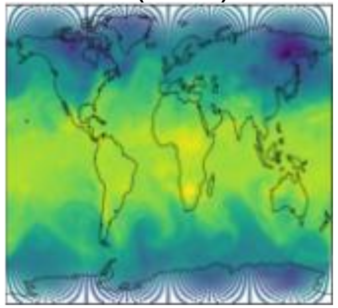


Graph attention



Graph attention

Output
Prediction:
X(t+3h)



Variables:
- Atmospheric composition variables
  - AODs, PMs, Reactive gases
  - Mixing ratio at pressure levels
- Upper-air variables at 13 pressure levels (t,v,u,w,z)
- Surface variables (temperature, winds, pressure, radiation)
- Static geographical features, location and time information as input forcing

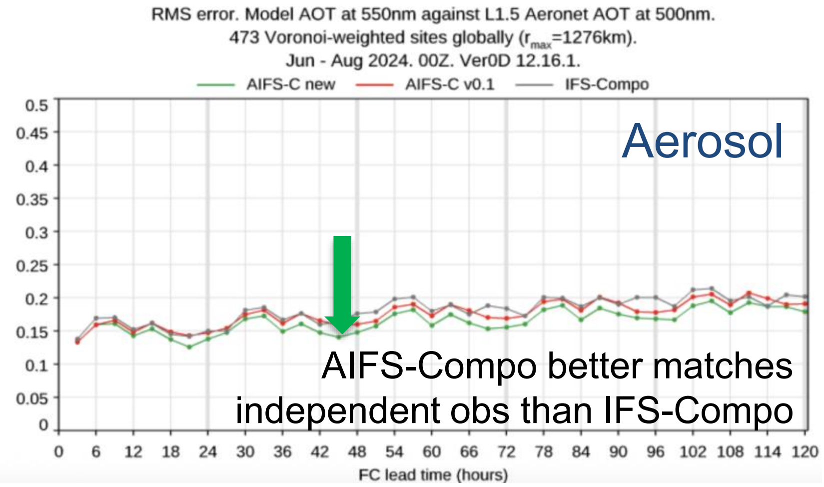
Training Scheme:
1. Train on EAC4
2. Fine-tune on operational analysis/forecast and lead times up to 36h

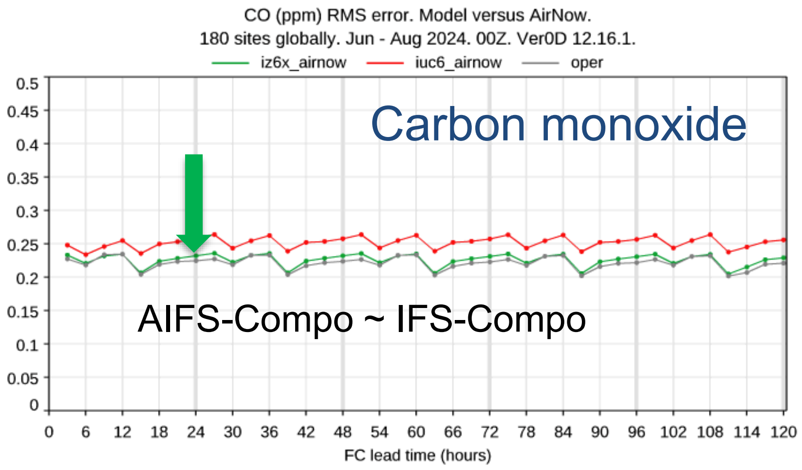
Several changes v0.1 -> vNew
- Moved from single-step input to multi-step input
- Bounding of all AC variables, including pressure levels
- Including newer years in pretraining/finetuning

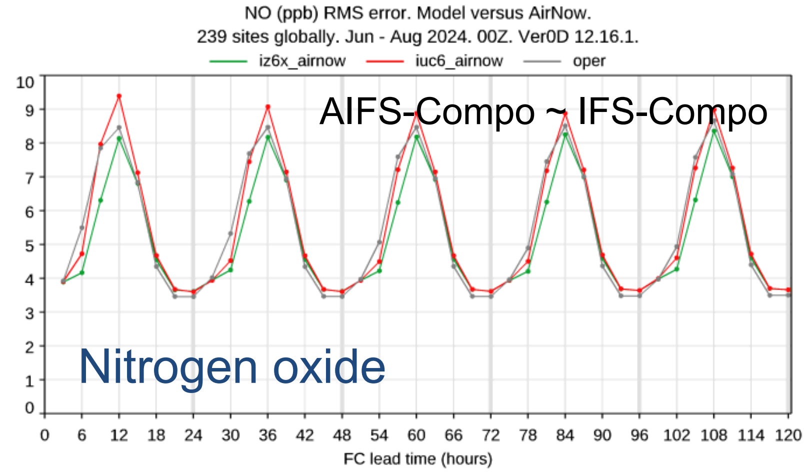
Implemented in anemoi

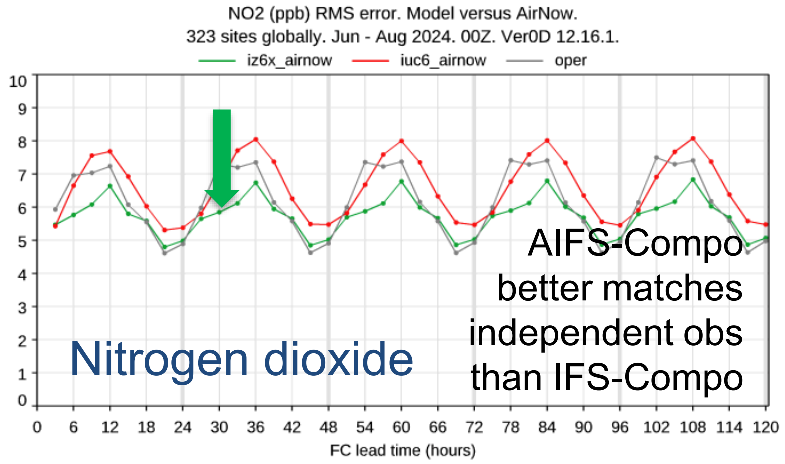
AIFS-Compo evaluation

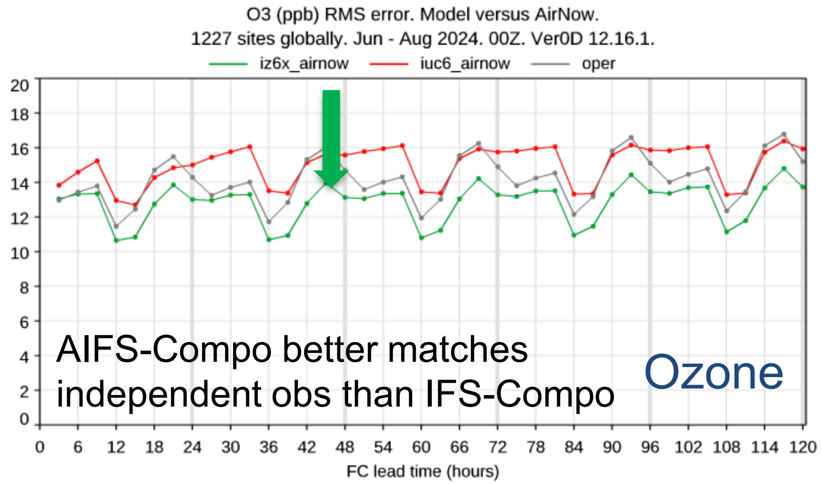
-- AIFS-Compo v0.1
-- AIFS-Compo new
-- IFS-Compo

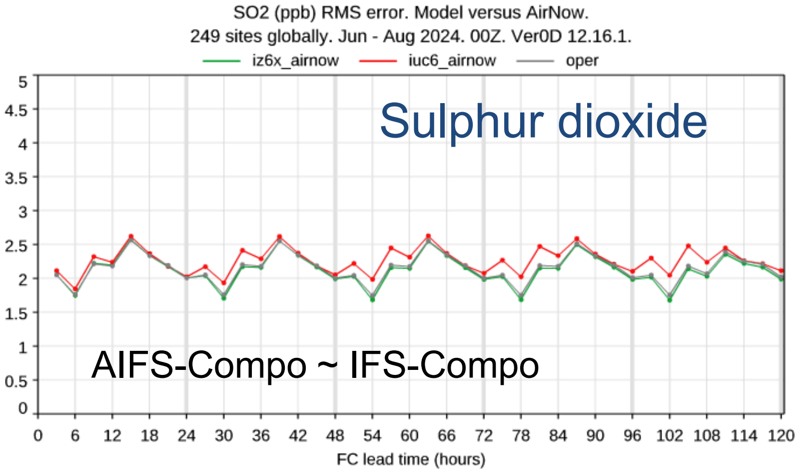








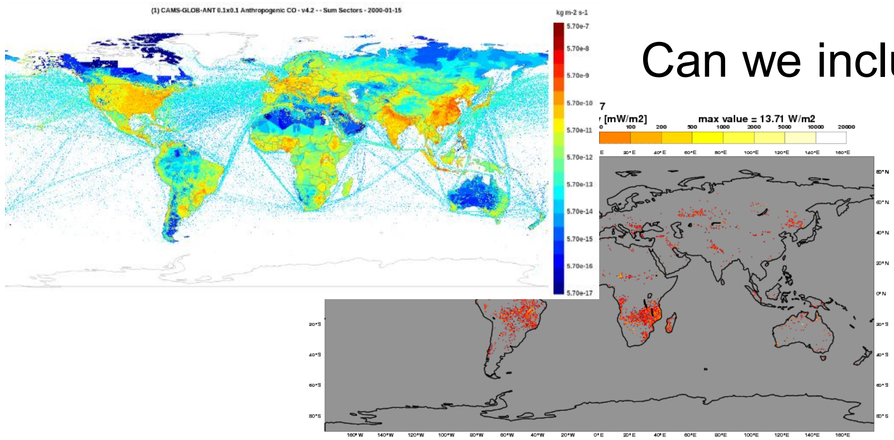




Results summary

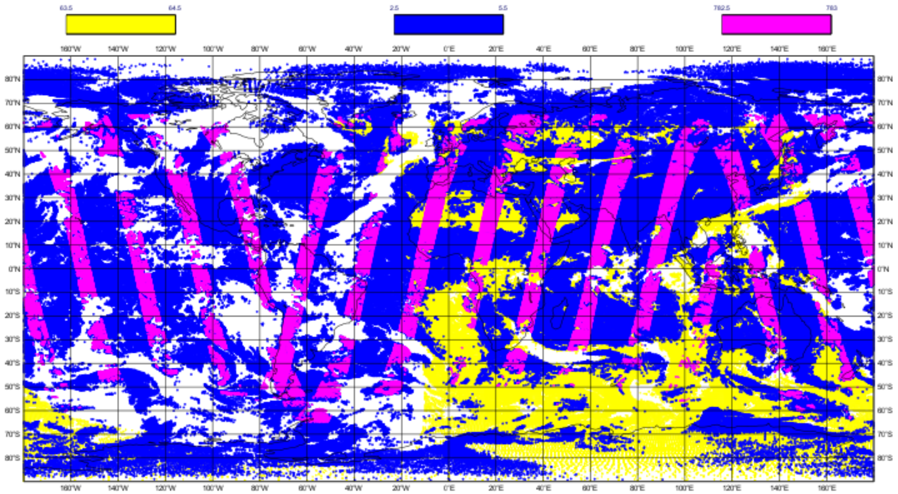
Good results for aerosols	Compared to observation AIFS-Compo beats IFS-Compo for AOD, PM2.5 and PM10 for almost all cases
Vnew leads to equal or better results for reactive gases	Reactive gases can match and, in some cases, beat the operational forecast NWP variables are less well predicted
20 days stability	Verified forecast up to 10days Stability of AI model up to 20days using 3h timesteps
Large speedup	Time to create a 3 hourly 5-day forecast AIFS-Compo: 0.76s on 1GPU IFS-Compo: 1000s on 8000CPUs

What does this mean for Data Assimilation for AC



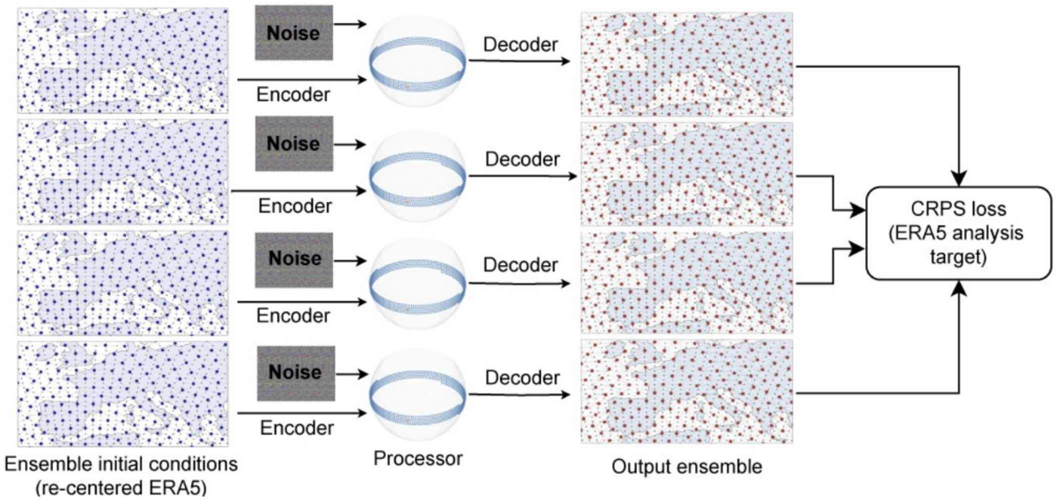
Can we include emissions in a machine learning approach?

CO: TROPOMI, MOPITT, IASI



Direct learning from observations – would this work with the limitations of atmospheric composition observations:

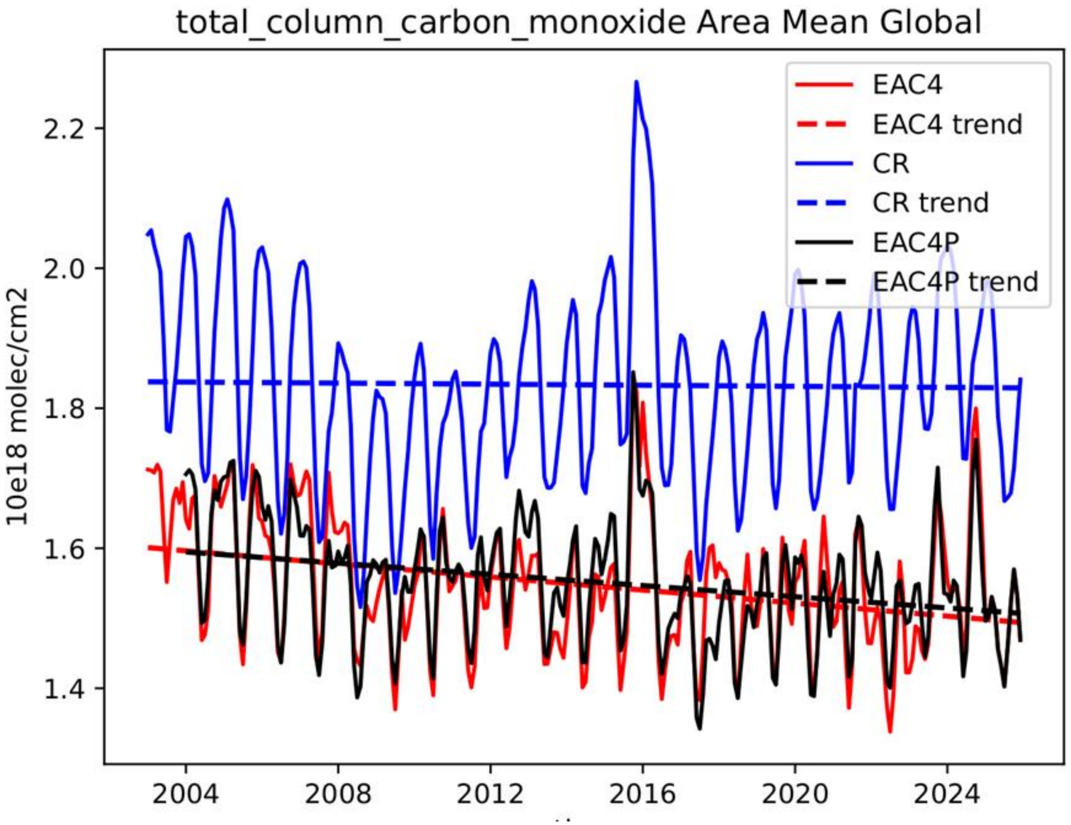
- Total column
- Limited spatial coverage in a 12hr cycle
- Importance of emissions

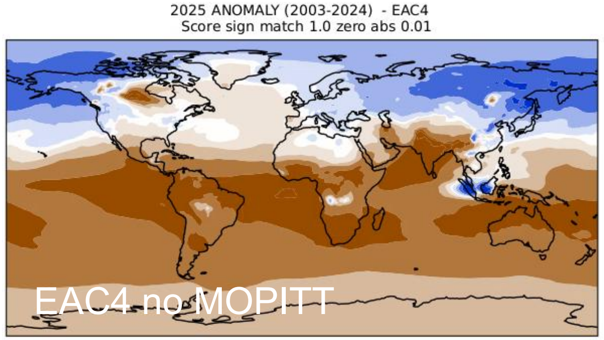


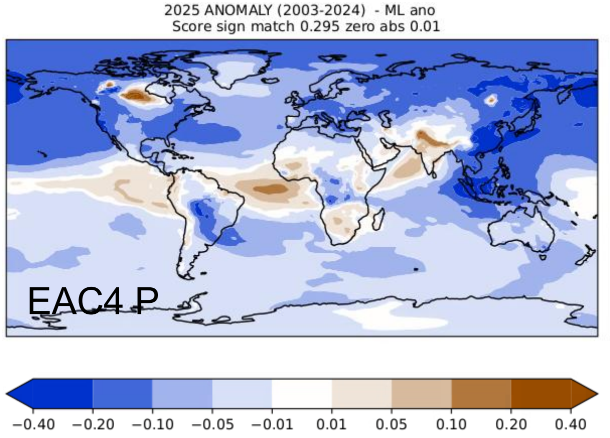
Background errors – Simulate an EDA to gain errors of the day for AC?

Carbon monoxide reanalysis

- Global monitoring of CO is done using the CAMS reanalysis (EAC4) long term assimilation cycling experiment
- Matching CTRL simulation (same model, emissions and meteorology) to assess the impact of obs
- EAC4 uses observations exclusively from MOPITT
- MOPITT was discontinued in January 2025 causing a shift in total column CO (TCCO)
- Monthly mean TCCO data was generated using a machine learning extension of EAC4:
    - Predictors: monthly-mean TCCO, total columns of formaldehyde from a control simulation (CR) from 2020-2025







2025 TCCO Anomaly

Harder P. and J. Flemming, Reconstructing Carbon Monoxide Reanalysis with Machine LearningCorrecting Carbon Monoxide with Machine Learning, submitted to arXive , 2026.

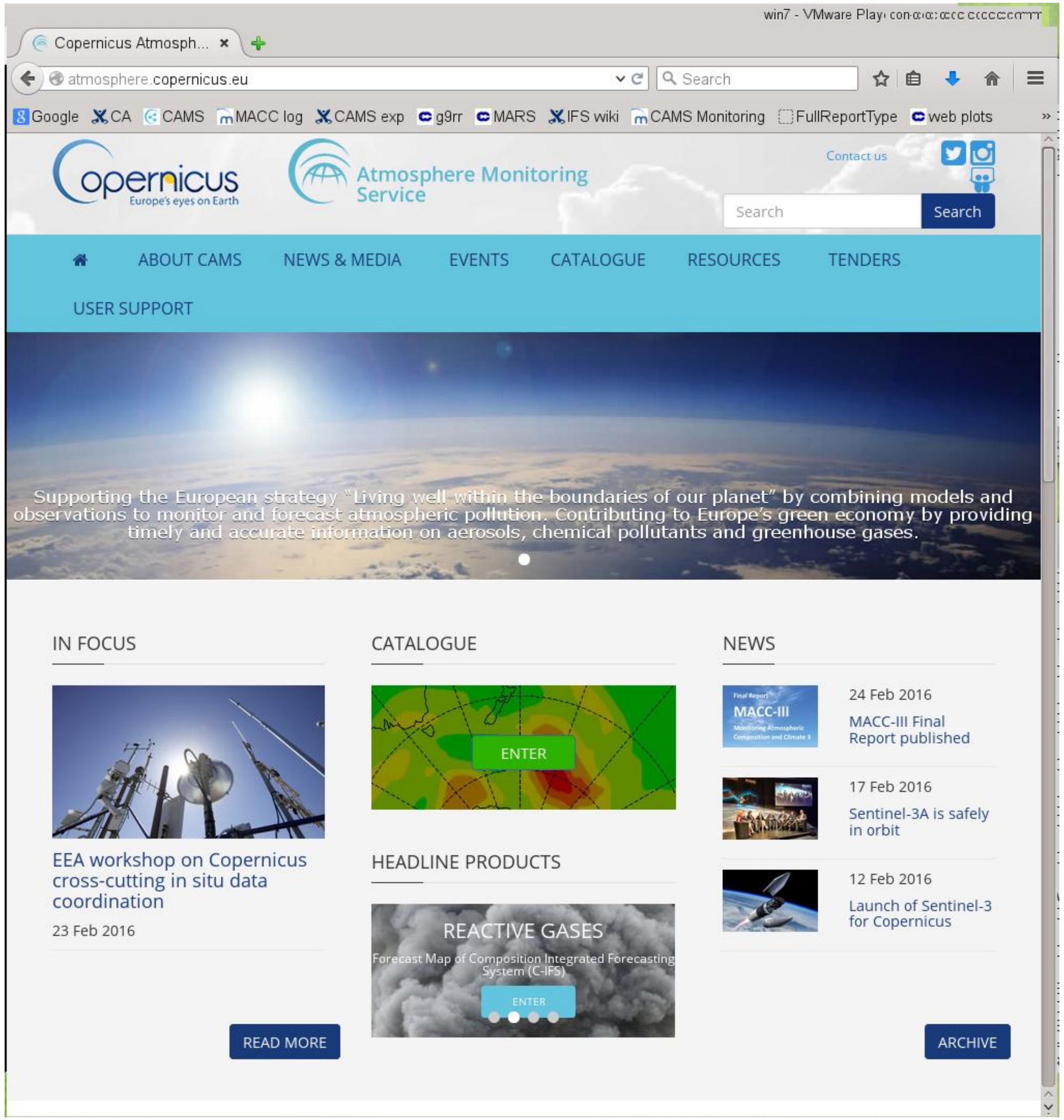
Summary

What we have seen today…

- Basic Data Assimilation theory is the same
- Particular challenges related to DA for atmospheric composition
  - Boundary conditions (emissions) as well as initial conditions
  - Mismatches between modelled and observed variables
  - Fast reactions and short lifetime of some species
- Atmospheric composition has the potential to improve various aspects of NWP
- Machine Learning can be used for AC forecasts in a similar manner to NWP
  - It can also be used to fill in gaps when observations are discontinued
- CAMS system produces useful Atmospheric Composition forecasts and analyses, freely available from atmosphere.copernicus.eu

More information about the environmental monitoring activities at ECMWF and how to access the data can be found on:

atmosphere.copernicus.eu



European Commission

ECMWF EUROPEAN CENTRE FOR MEDIUM-RANGE WEATHER FORECASTS

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