Atmosphere Monitoring

Satellite data assimilation of atmospheric composition

Melanie Ades (ECMWF)

Contributions from: Nicolas Bousserez, Antje Inness, Johannes Flemming, Richard Engelen, Peter Hill, Vincent Huijnen, Samuel Quesada Ruiz, Ziga Zaplotnik

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European Commission
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Why atmospheric composition at an operational weather prediction centre?

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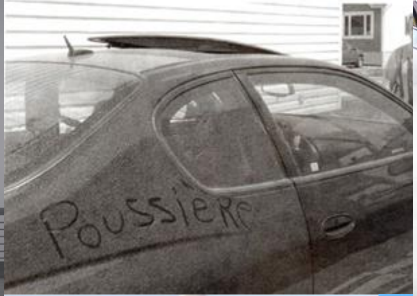
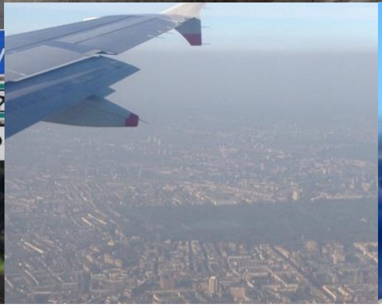
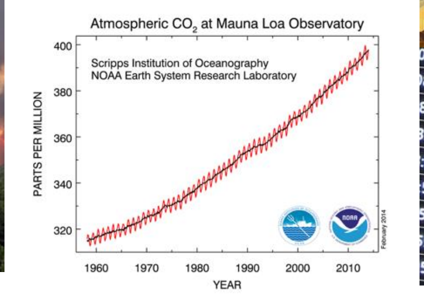
- Poor air quality is a major public health issue in many countries.
- Local authorities need accurate and timely information to implement effective air pollution mitigation measures.
- Accurate air quality forecasts require accurate transport models.
- Can leverage sophisticated data acquisition infrastructures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







Why this lecture?

- Basic data assimilation theory is the same for atmospheric composition, but…
  - Radiance assimilation is not always feasible (yet)
  - Atmospheric composition data assimilation is much more influenced by additional factors such as emissions and chemistry than by the initial values
  - With many species not being observed, the problem is even more underdetermined than the standard NWP case
- Atmospheric composition impacts the basic NWP problem as well

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1. Copernicus Atmosphere Monitoring Service (CAMS)

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What the Copernicus Atmosphere Monitoring Service has to offer

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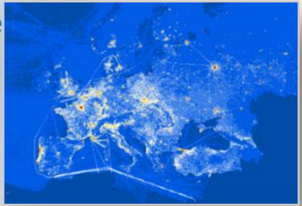

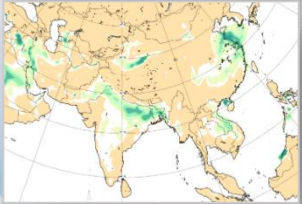

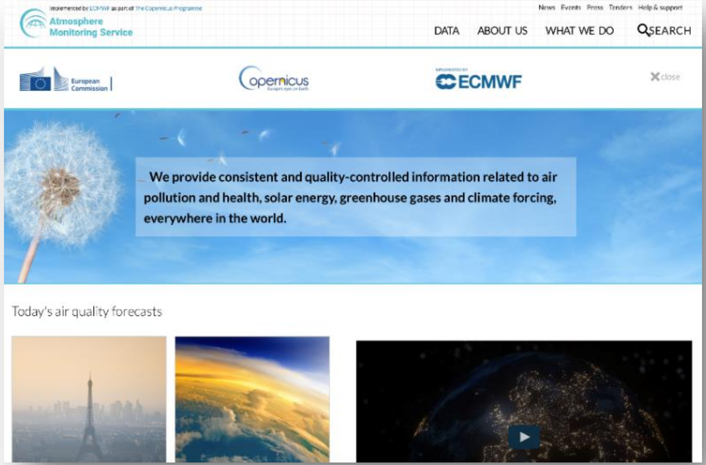

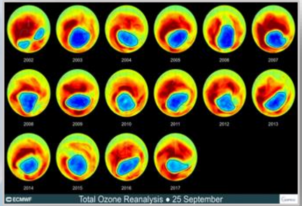

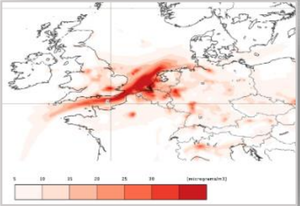

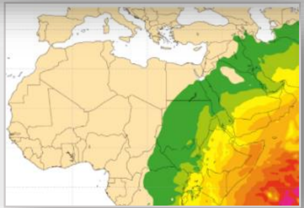

The CAMS portfolio includes Earth Observation based information products about:

- 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.
- reanalysis of atmospheric composition (back to 2003)

Quarterly validation reports of global and regional outputs.

This is done by assimilating atmospheric composition data into the IFS (in addition to meteorological observations)

https://atmosphere.copernicus.eu

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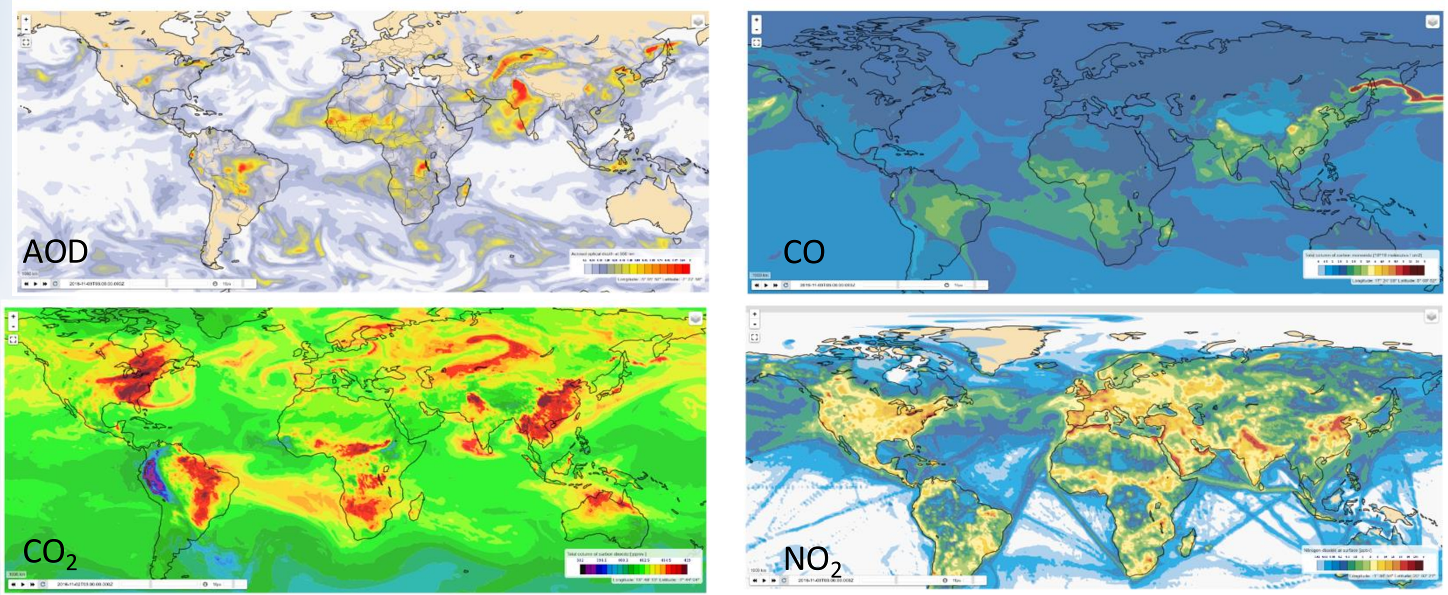
C A M S G l o b a l S y s t e m



40km horizontal resolution at 137 model levels; two 5-day forecasts at 00z and 12z UTC each day

- **Aerosols (AOD and concentrations): e.g. biomass burning, dust, sea-salt, sulphate, …**
- **Reactive gases: CO, HCHO, NO_2, O_3, SO_2**

9km horizontal resolution at 137 model levels; one 5-day forecast per day (CO_2, CH_4, linear CO)

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2. Data assimilation methodology for atmospheric composition

Cost function

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

Analysis: x that minimizes cost function

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

Cost function

J_b
Background term

J_o
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 constrained 4D-Var** includes a model error term – being 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

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

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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Data assimilation methodology

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Chemical module

GHG module

Aerosol module

Chemical Module

TM5 (CB05) & BASCOE
100+ species and reactions,
Photolysis, dry and wet deposition

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Data assimilation methodology

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

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

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aerosol mixing ratio

Chemical module

GHG module

Aerosol module

Greenhouse Gas Module

CHTESSEL
Photosynthesis & ecosystem respiration model
Diagnoses the gross primary production of CO2 by plants and release of CO2 by soil

CH4 comes from prescribed emissions and climatological loss

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Data assimilation methodology

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

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

Control variables

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Atmospheric Composition

ozone
carbon monoxide
nitrogen dioxide
formaldehyde
sulphur dioxide

carbon dioxide
methane

aerosol mixing ratio

Chemical module

GHG module

Aerosol module

Aerosol bin scheme

16 aerosol-related prognostic variables:
3 bins sea-salt, 3 bins dust, Black carbon, Organic matter, Sulphate,
2 bins Nitrate, Ammonium,
Secondary Organic Aerosols

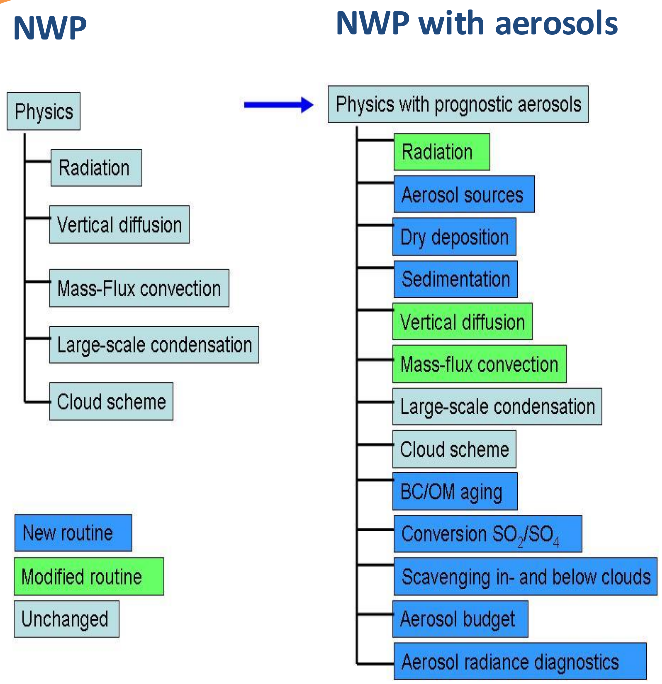
Emissions, dry and wet deposition, sedimentation

Combining the AC and NWP models

- Atmospheric composition models can be run coupled to NWP or fully integrated.

IFS

In the IFS the atmospheric composition and NWP models are fully integrated



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

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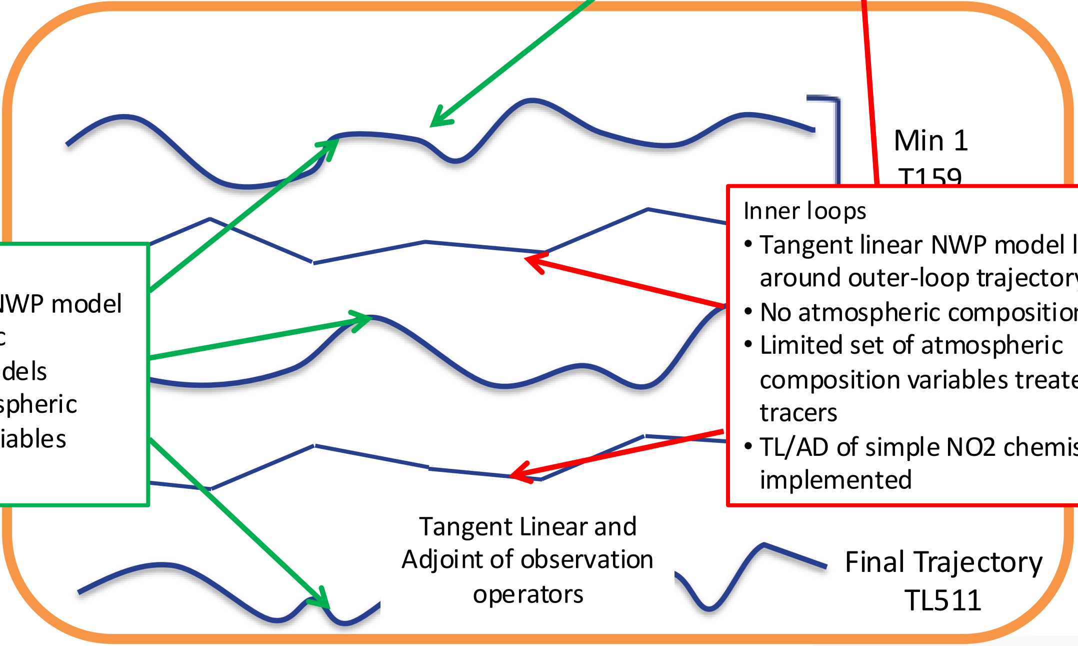
Data assimilation methodology

Incremental 4DVar:

$$J(\delta\mathbf{x}) = \frac{1}{2}\delta\mathbf{x}^{\mathrm{T}}\mathbf{B}^{-1}\delta\mathbf{x} + \frac{1}{2}\sum_{i=0}^{n}(\mathbf{H}_i\delta\mathbf{x}(t_i) - \mathbf{d}_i)^{\mathrm{T}}\mathbf{R}_i^{-1}(\mathbf{H}_i\delta\mathbf{x}(t_i) - \mathbf{d}_i)$$

Resolutions of CAMS NRT system



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

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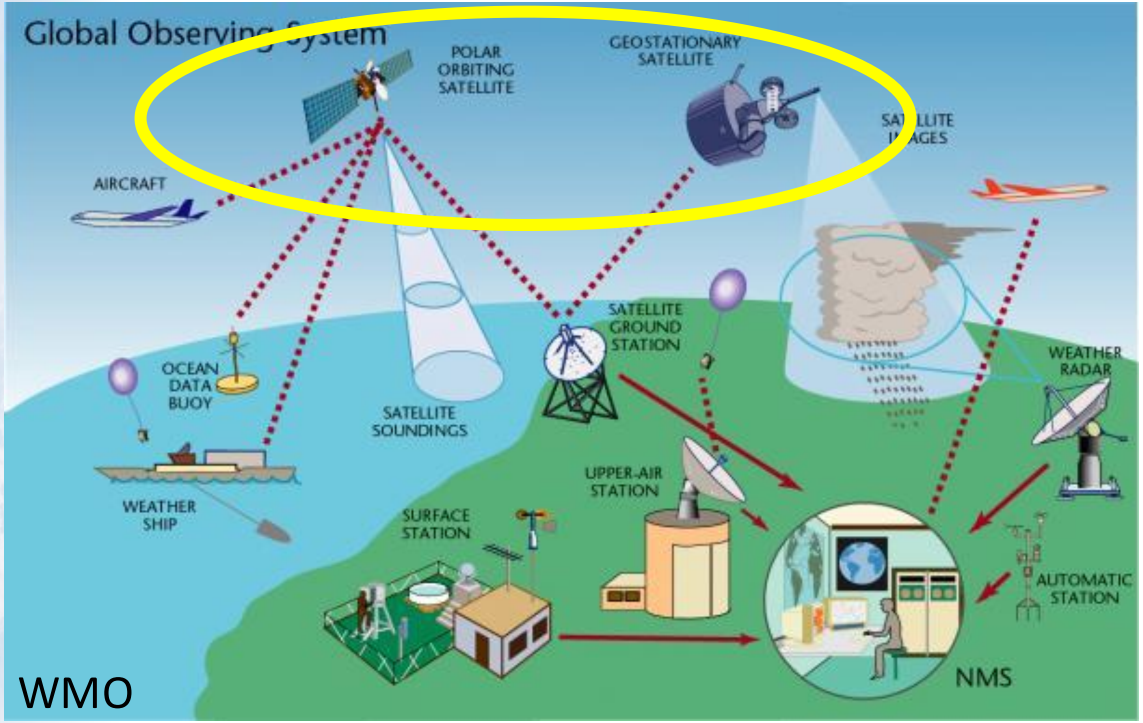
3. Observations of atmospheric composition

Global observing system



We want to provide information about near-surface air quality

- CAMS assimilates satellite retrievals of atmospheric composition
- CAMS uses ground-based & aircraft data and satellite retrievals for validation

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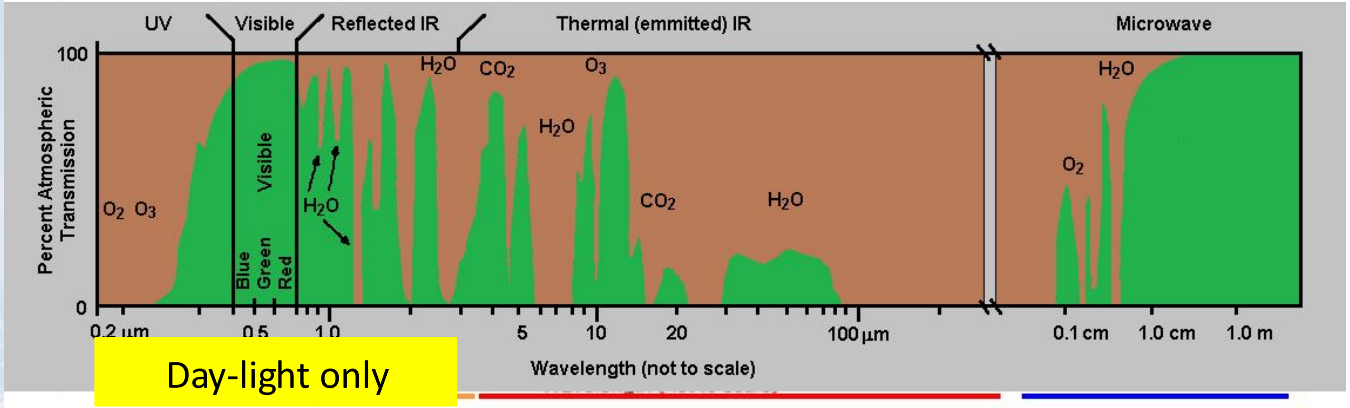
Spectral signature of trace gases

NIR, SWIR



O_3
H_2O
NO_2
SO_2
H_2CO, $C_2H_2O_2$
IO
BrO

AOD MODIS

GOME, GOME-2, SCIAMACHY,
OMI *at nadir* TROPOMI
SCIAMACHY, OSIRIS *at limb*

CO_2
CH_4
CO

SCIAMACHY,
GOSAT, OCO *at nadir* TROPOMI

H_2O
CO_2
CH_4
N_2O
O_3
CO
HNO_3
NH_3
CFC11, CFC12, …
CH_3OH, HCOOH, C_2H_2, C_2H_6,…
+ isotopologues

TES, AIRS, IASI, MOPITT
at nadir
MIPAS, ACE *at limb*

O_2
H_2O, OH, HO_2
HNO_3
HCl, BrO, ClO, HOCl
O3
CO
HCN, CH_3CN

DMR, MLS *at limb*

Credit: M. Van Roozendael

A C O b s e r v a t i o n s u s e d i n C A M S

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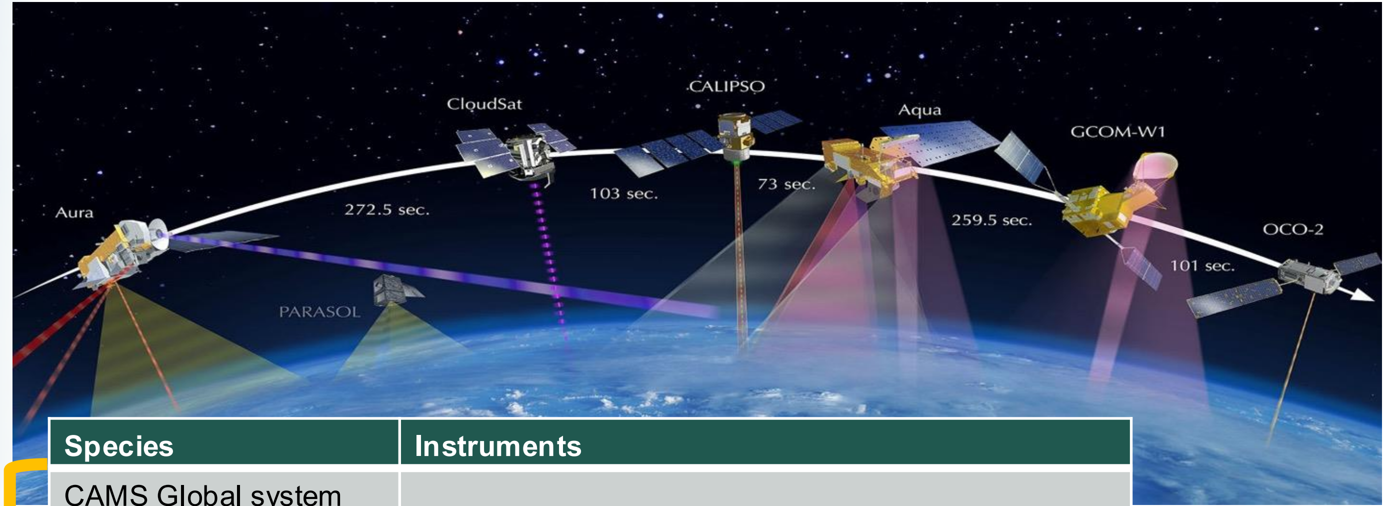

All from LEOs

Species	Instruments
CAMS Global system	
O_3	OMI, SBUV, GOME-2, MLS, OMPS, S5p
CO	MOPITT, IASI, S5p
NO_2	GOME-2, S5P
Aerosol	MODIS, PMAp, VIIRS, S3
CO_2	GOSAT, IASI, OCO-2
CH_4	GOSAT, IASI, S5P
GFAS fire emissions	MODIS, SEVIRI*, VIIRS, Sentinel-3, GOES-E/W*, HIMAWARI-8*

Radiances versus retrievals

L2 retrievals generally use same methodology as data assimilation - minimize a cost function that contains the observations and some a-priori constraint:

$$J(\mathbf{x}) = \frac{1}{2}(\mathbf{x} - \mathbf{x}_r^b)^{\mathrm{T}} \mathbf{B}_r^{-1} (\mathbf{x} - \mathbf{x}_r^b) + \frac{1}{2}[\mathbf{y}^o - H(\mathbf{x})]^{\mathrm{T}} \mathbf{R}^{-1} [\mathbf{y}^o - H(\mathbf{x})]$$

$$\text{Simplified solution: } \mathbf{x}_r = \alpha \mathbf{x} + \beta \mathbf{x}_r^b$$

The retrieved value will be biased relative to the assimilation model background, when the prior information is different from the model background.

This bias will have a vertical structure based on the vertical sensitivity of the observations.

How do we use retrievals in 2023?

Retrieval $\mathbf{x}_r$ can be written (after linearization) as:

$$\mathbf{x}_r = \mathbf{x}_r^b + \mathbf{A}(\mathbf{x} - \mathbf{x}_r^b) + \varepsilon = \mathbf{A}\mathbf{x} + (\mathbf{I} - \mathbf{A})\mathbf{x}_r^b + \varepsilon$$

With a-priori $\mathbf{x}_r^b$, error covariance matrix $\mathbf{S}_r$ and averaging kernel **A**:

$$\mathbf{S}_r = \left(\mathbf{K}^T\mathbf{R}^{-1}\mathbf{K} + \mathbf{B}^{-1}\right)^{-1}$$

$$\mathbf{A} = \mathbf{S}_r\mathbf{K}^T\mathbf{R}^{-1}\mathbf{K}$$

R: observation error covariance matrix
B: prior error covariance matrix
K: weighting function

The averaging kernel **A** describes the vertical structure of the impact of the a priori information.

Example MOPITT CO Averaging Kernels

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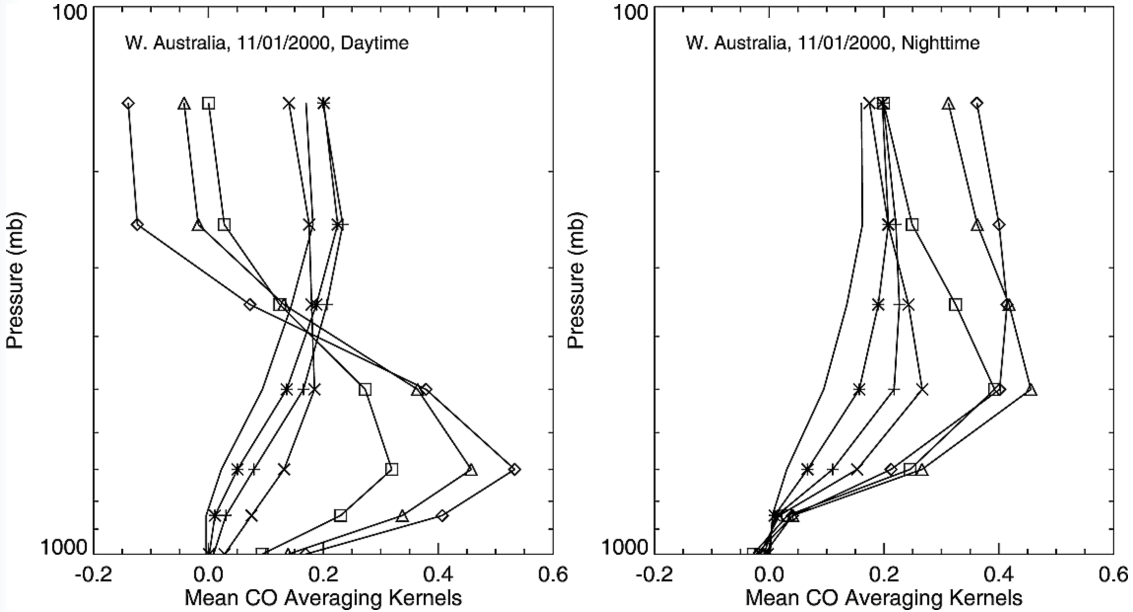

From: Deeter et al. (2003) JGR

- Diurnal variations of Tsurf affect retrieval over land.
- CO near surface more detectable during day, AKs shift downwards
- Diurnal variability of AKs largest over e.g. deserts, smallest over sea
- If AKs are not used this can introduce an artificial diurnal CO cycle in the analysis

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Assimilating retrievals: Column retrieval example

We can make use of the averaging kernel **A** in the observation:

$$d = y - H(\mathbf{x}_m) = \mathbf{x}_r^b + \mathbf{A}(\mathbf{x} - \mathbf{x}_r^b) + \varepsilon - H(\mathbf{x}_m)$$

Without averaging kernels in observation operator

$$d = y - \hat{H}(\mathbf{x}_m) = \mathbf{x}_r^b + \mathbf{A}(\mathbf{x} - \mathbf{x}_r^b) + \varepsilon - (\mathbf{x}_r^b + \mathbf{A}(H(\mathbf{x}_m) - \mathbf{x}_r^b))$$
$$= \mathbf{A}(\mathbf{x} - H(\mathbf{x}_m)) + \varepsilon$$

With averaging kernels in observation operator

We remove the influence of the a-priori profile if we use the averaging kernel to sample the model profile according to the assumptions made in the retrieval.

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Issues

- Total column retrievals come with integrated averaging kernels; some information is lost
- Profile retrievals with full averaging kernels and retrieval errors can become difficult to handle
- Not all retrieval methods allow the estimation of an averaging kernel; e.g., neural networks
- Not all data providers use the same definition of averaging kernel in their data files
- Many different versions of the observation operator needed to deal with all variations
- We use:
  - Reactive gases: Profiles, columns with and without averaging kernels
  - Aerosols: Columns without averaging kernels, profiles being tested
  - Greenhouse gases: Radiances and columns with averaging kernels

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Assimilating retrievals: summary

- Easier
- No radiative transfer model for some of the species of interest
- Bad experiences with radiance assimilation:

  Combination of model bias and VarBC in CO_2 data assimilation from AIRS and IASI radiances caused artificial long-term trend. Tests with IASI/AIRS ozone radiance assimilation led to degraded tropospheric ozone in CAMS

- Retrieval teams can focus their expertise fully on specific observation
- Good communication between data providers and data assimilation users needed
- Good characterization of retrieval is crucial
  - Averaging kernels
  - A priori
  - Error estimates
  - Quality flags

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4. Emissions and emission inversion

Initial condition vs boundary problem

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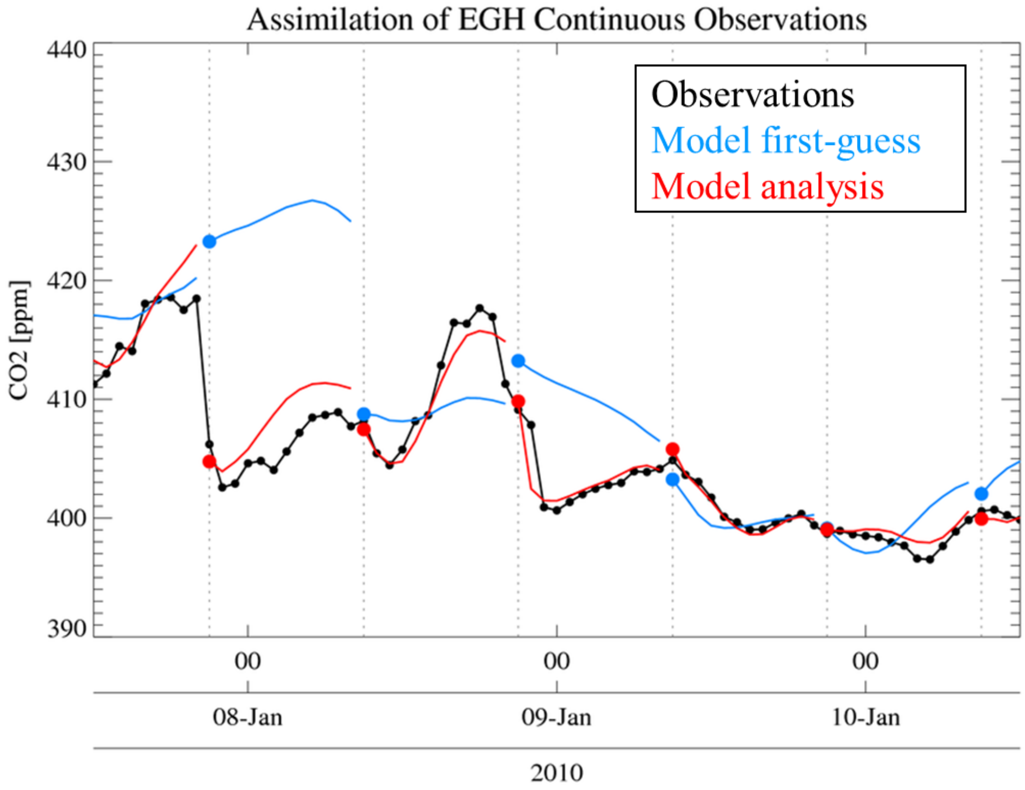

- NWP 4D-Var is mostly defined as an initial value problem. Only initial conditions are changed and model error is relatively small.
- AC modelling depends on initial state and surface fluxes
- Large part of chemical system not sensitive to initial conditions because of chemical equilibrium, but dependent on other parameters (e.g. emissions, deposition, reaction rates, …) which all might have errors

Examples of emissions

TNO European anthropogenic NOx emissions

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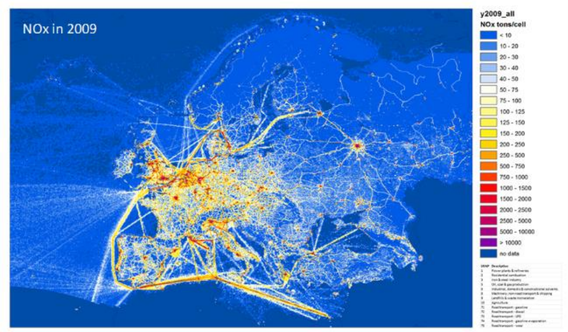
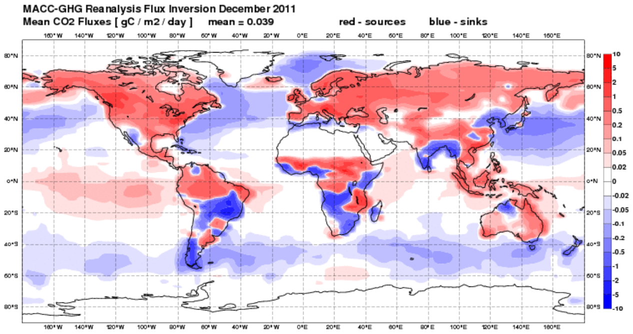
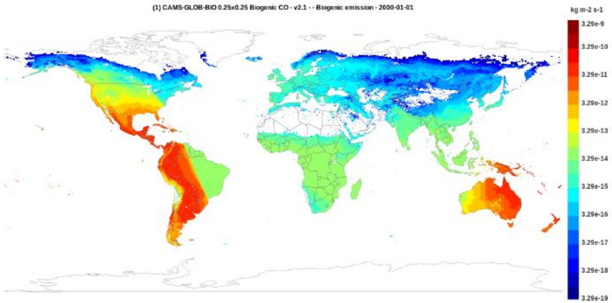


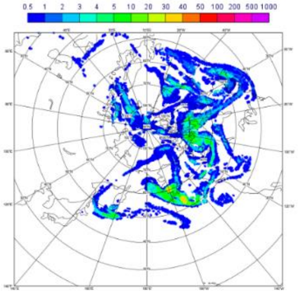
CO2 fluxes



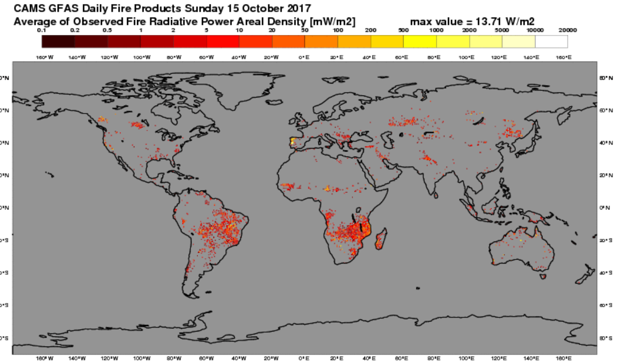
CAMS_GLOB biogenic CO emissions



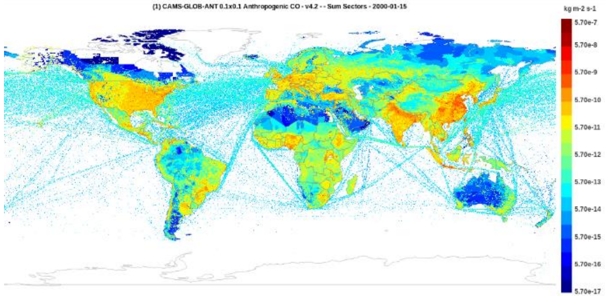
Volcanic SO2



Biomass burning, 15 October 2017



CAMS_GLOB anthropogenic emissions



Short-lived memory of NO2 assimilation

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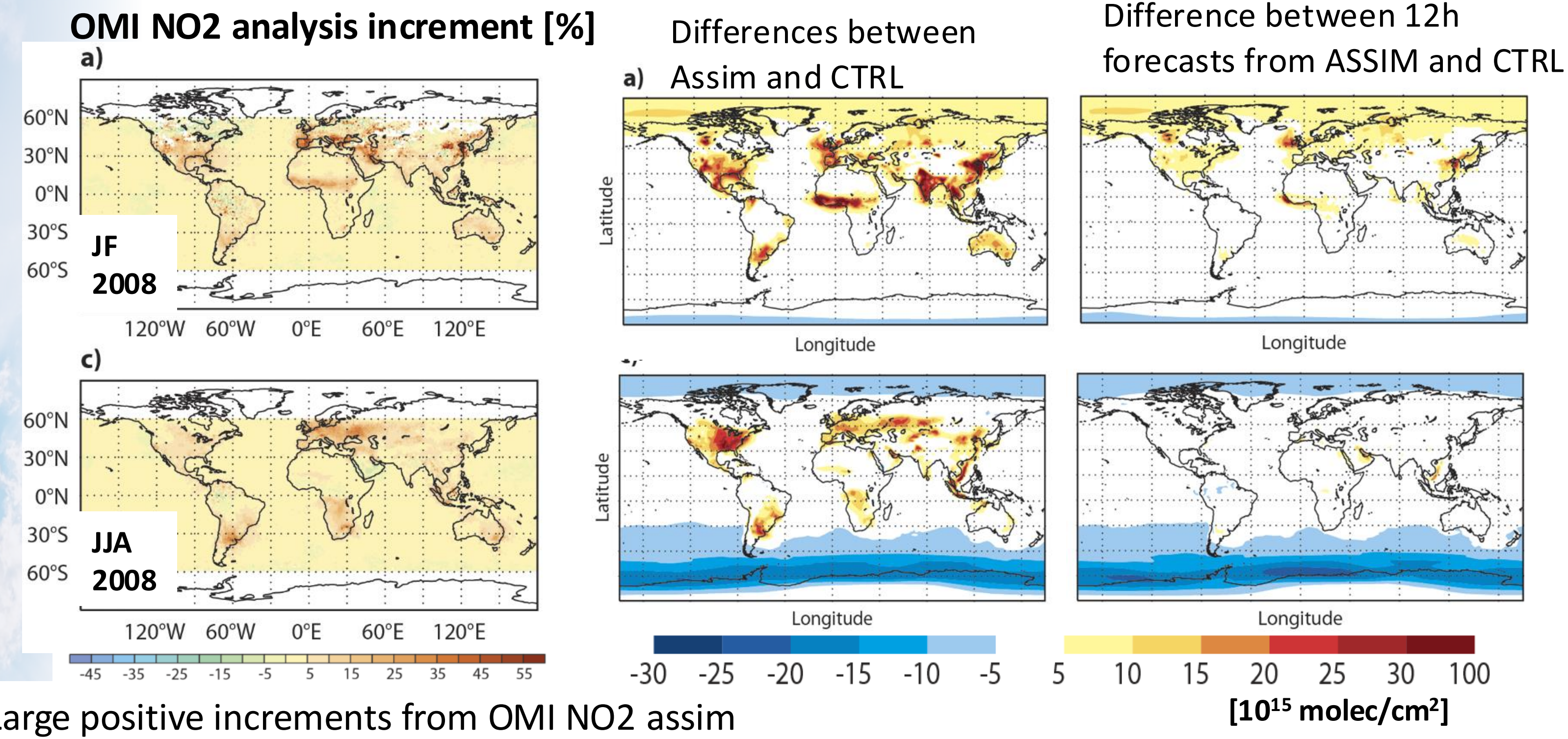

- Large positive increments from OMI NO2 assim
- Large differences between analyses of ASSIM and CTRL
- Impact is lost during subsequent 12h forecast
- Constraining emissions (in addition of IC) would give a better initial state and persistence of forecast improvements throughout the DA window

Inness et al. (2015, ACP)

Emissions

- Emissions are one of the major uncertainties in composition modeling (can not be measured directly)
- The compilation of emissions inventories is a labour-intensive task based on a wide variety of socio-economic and land use data
- Trends are applied to inventories from previous years to produce future emission datasets
- Some emissions can be “modeled” based on wind (dust and sea salt aerosol) or temperature (biogenic emissions)
- Some emissions can be observed indirectly from satellites instruments (Fire radiative power, burnt area, volcanic plumes)
- “Inverse” methods can be used to correct prior emission estimates using observations of concentrations and models

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How to improve?

Adjust emissions as well as concentrations

$J(x) = (x$ ... $) +$ ... $R_i^{-1}(y_i - H_i[x_i])$

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

+

Additional control variables

Emissions

nitrogen dioxide
carbon monoxide
carbon dioxide
methane

All these species are dominated by emissions – changing initial conditions is not enough

Include as a scaling factor adjustment to the prior (inventory-based) emissions

Increases the computation time

Joint state/emissions 4D-var inversion system

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J_b: background constraint for x

J_p: constraint for emission scaling factors

$$J(x,p) = \underbrace{(x - x_b)^T B^{-1}(x - x_b)}_{J_b} + \underbrace{(p - p_b)^T {B_p}^{-1}(p - p_b)}_{J_p}$$

State control vector

Parameter (e.g. scaling factors)

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

J_o: observation constraint

- Joint optimisation of emissions and initial conditions
- Optimized emissions e.g. CO_2, CH_4, CO & 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 contrain CO_2 emissions

Credit: Nicolas Bousserez

4D-VAR NOX inversion results

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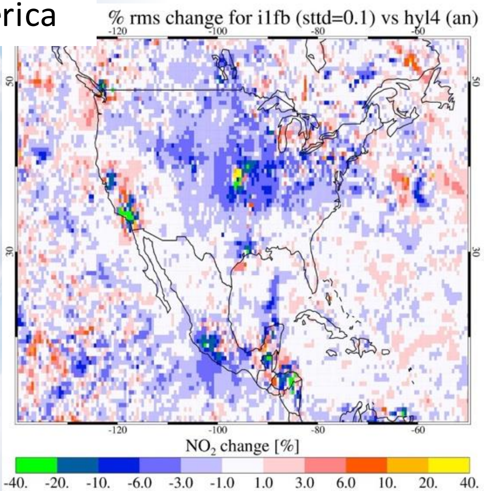
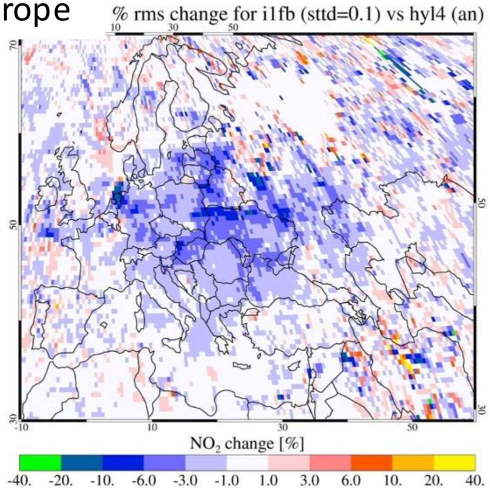
- Evaluation of 24h forecast of NO_2 columns against TROPOMI NO_2 observations.
- Decrease in rms error > 50% over some areas in Eastern Asia and North America.
- Average decrease in rms error of about 5-10% over Europe.
- NOx and CO emission estimates will be used to constrain CO_2 emissions (HE CORSO project).

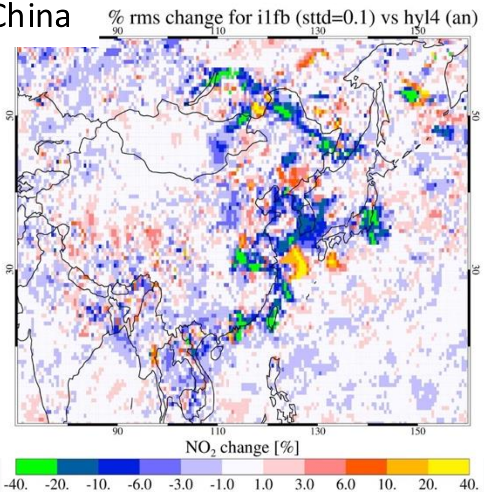
N-America



Europe



China



Credit: Vincent Huijnen, KNMI

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5. Potential issues when assimilating AC satellite data

Example of satellite observation coverage

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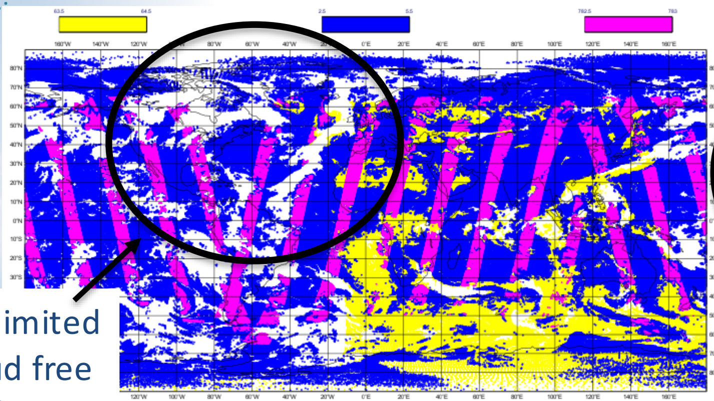
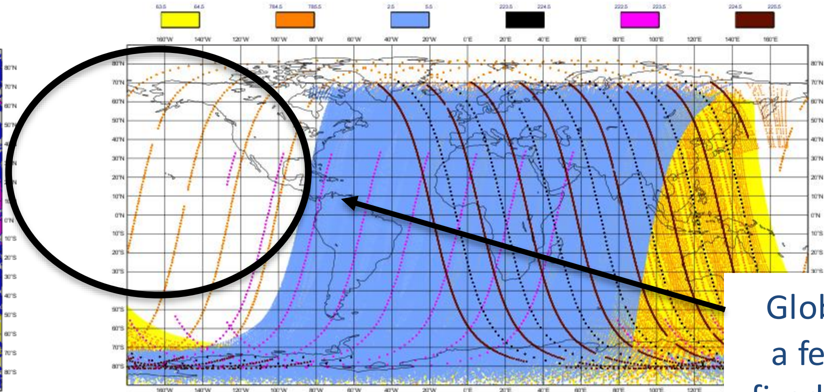
CO: TROPOMI, MOPITT, IASI



Often limited to cloud free conditions

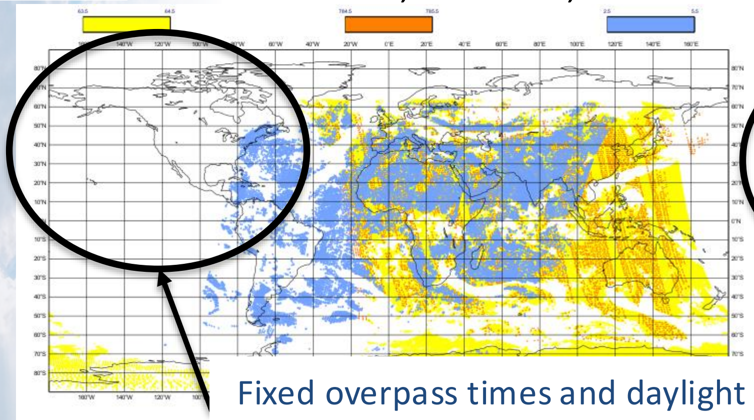
O3: TROPOMI, GOME-2,OMI,SBUV,OMPS,MLS



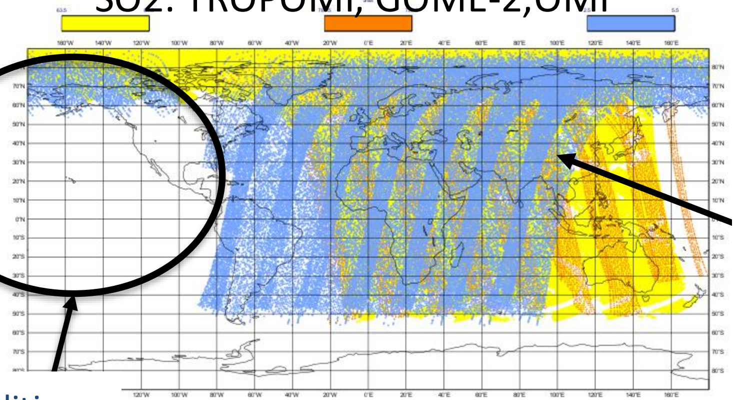
12-hour analysis cycle

Global coverage in a few days (LEO) – fixed overpass time

NO2: TROPOMI, GOME-2,OMI



SO2: TROPOMI, GOME-2,OMI



Total or tropospheric columns

Fixed overpass times and daylight conditions only (UV-VIS) -> no daily maximum/cycle

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.

Atmosphere Monitoring

Mismatch between modelled and observed variables

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

Total column and profile observations

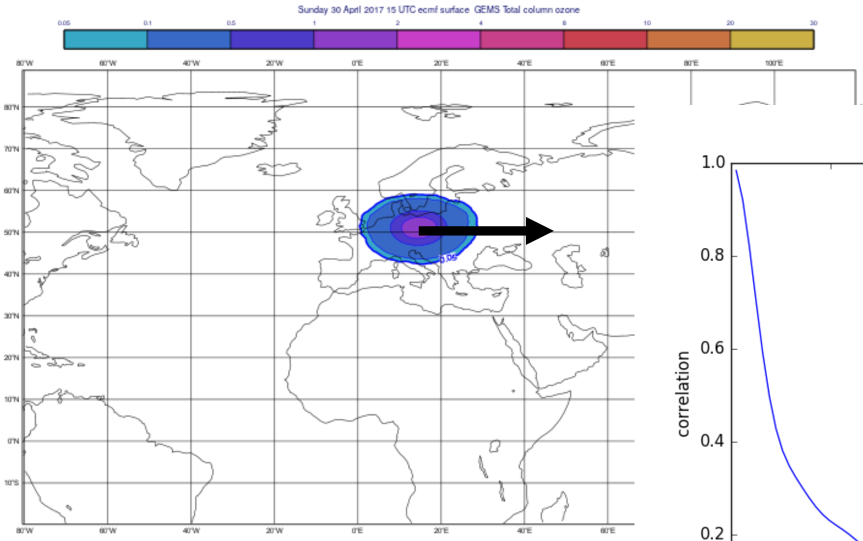
Total or tropospheric column observations

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

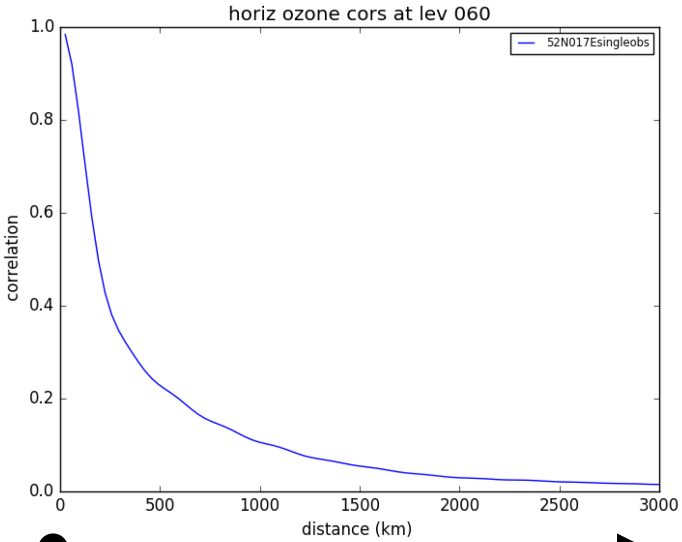
Even for those species that are observed, it is often only total column data that are available.

Limited information content: Total column

Increment from one TC ozone retrieval

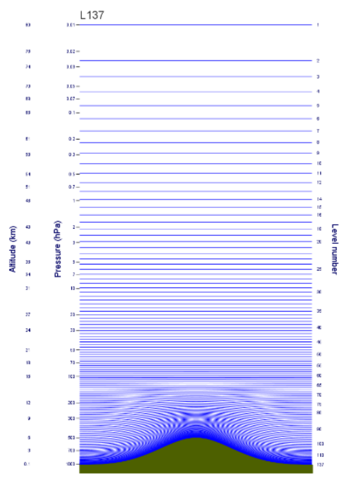


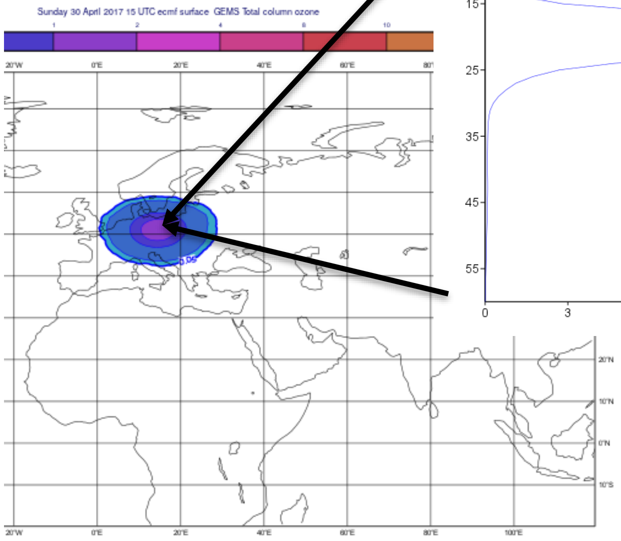
Increment created by a single ozone observation of 375 DU, 10 DU higher than background

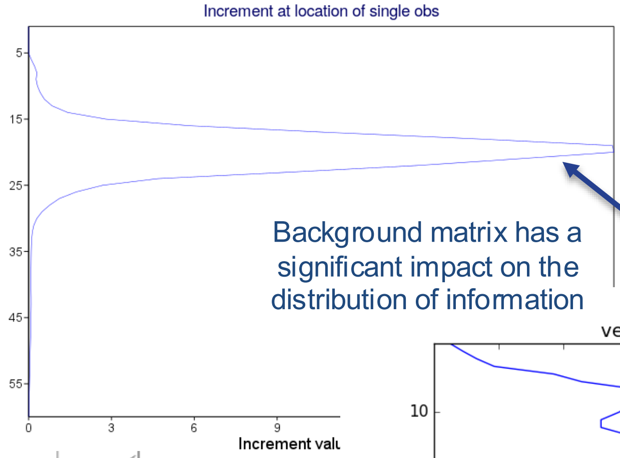


Horizontal correlation from the B-matrix that spreads the information from the single observation in the horizontal

Increment from one TC ozone retrieval



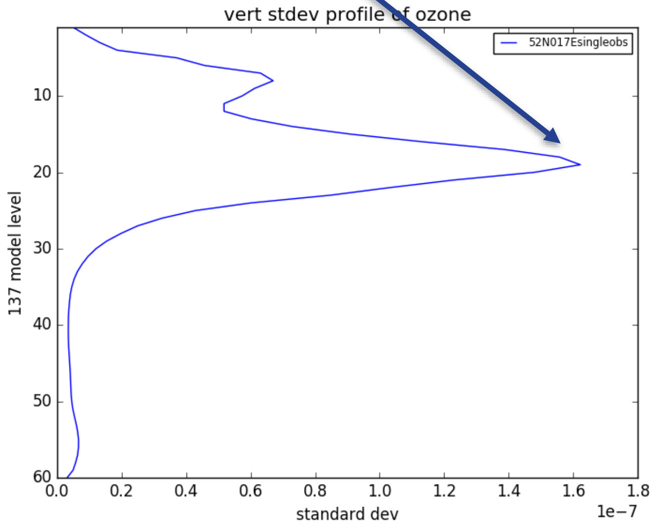




Vertical profile of the increment at the observation location

~35 hPa

Background matrix has a significant impact on the distribution of information

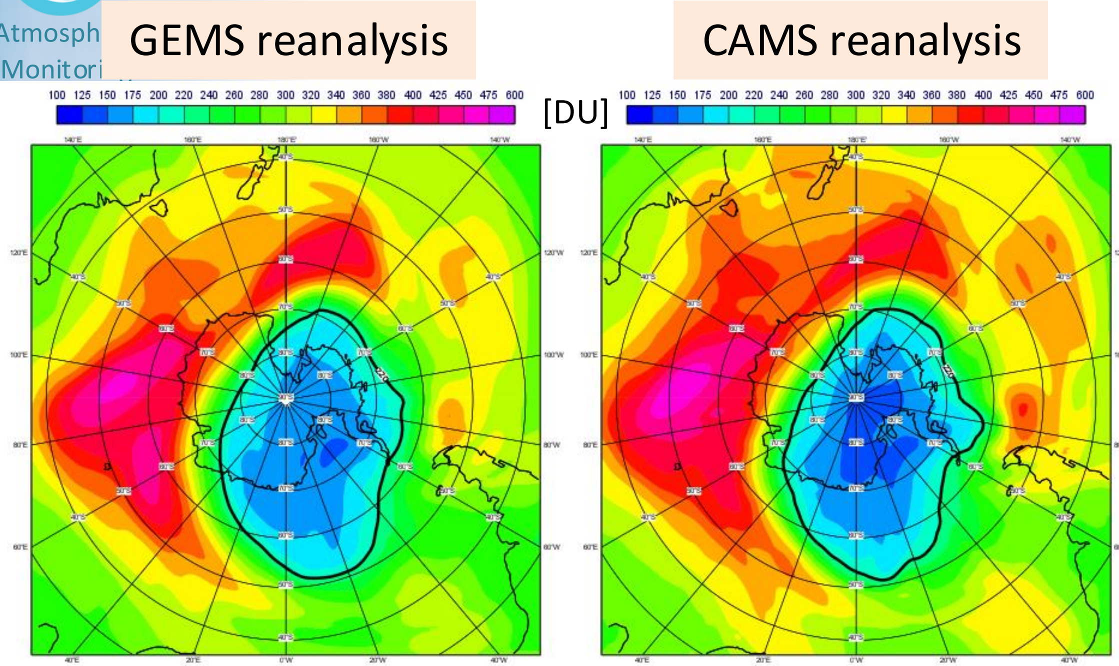


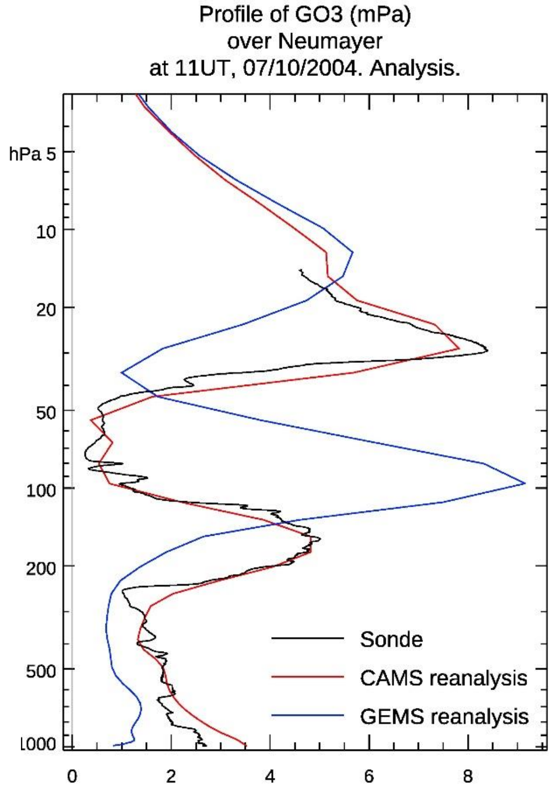
Increment created by a single ozone observation of 375 DU, 10 DU higher than background

Standard deviation from the background matrix at the observation location

Formulation of the B-matrix is very important for AC

An extreme example: Ozone 7 October 2004





Sonde launched by AWI

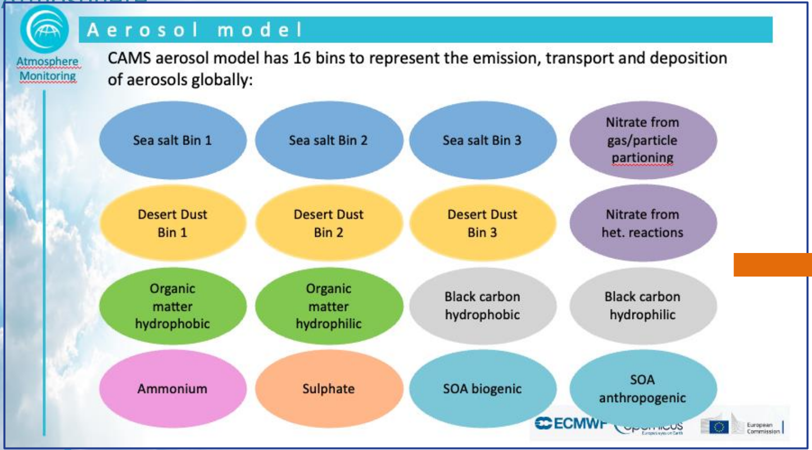
- Similar TCO3 analysis from (old) GEMS reanalysis and CAMS reanalysis
- Huge differences between corresponding O3 profiles
- No profile data (MIPAS, MLS) were assimilated in GEMSRA in Oct 2004 and model had a large O3 bias leading to very bad vertical O3 analysis profiles
- Shows importance of using limb sounding data for O3 analysis

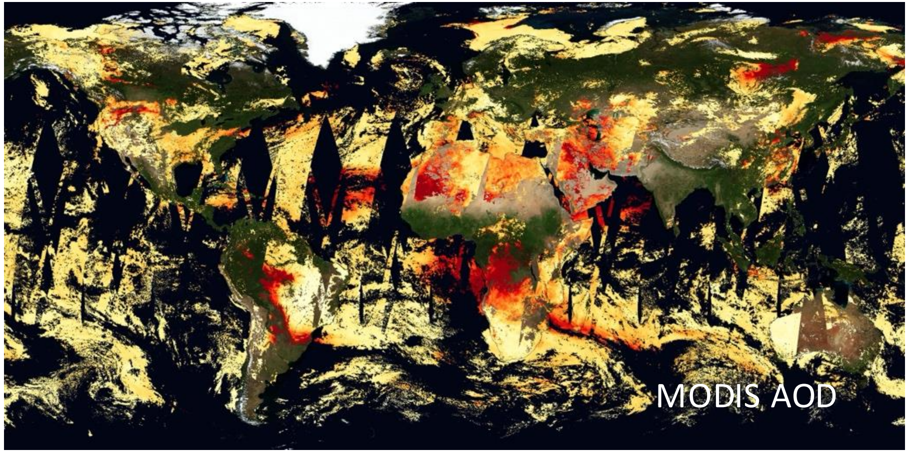
Aerosol model

CAMS aerosol model has 16 bins to represent the emission, transport and deposition of aerosols globally:

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

Aerosol observations

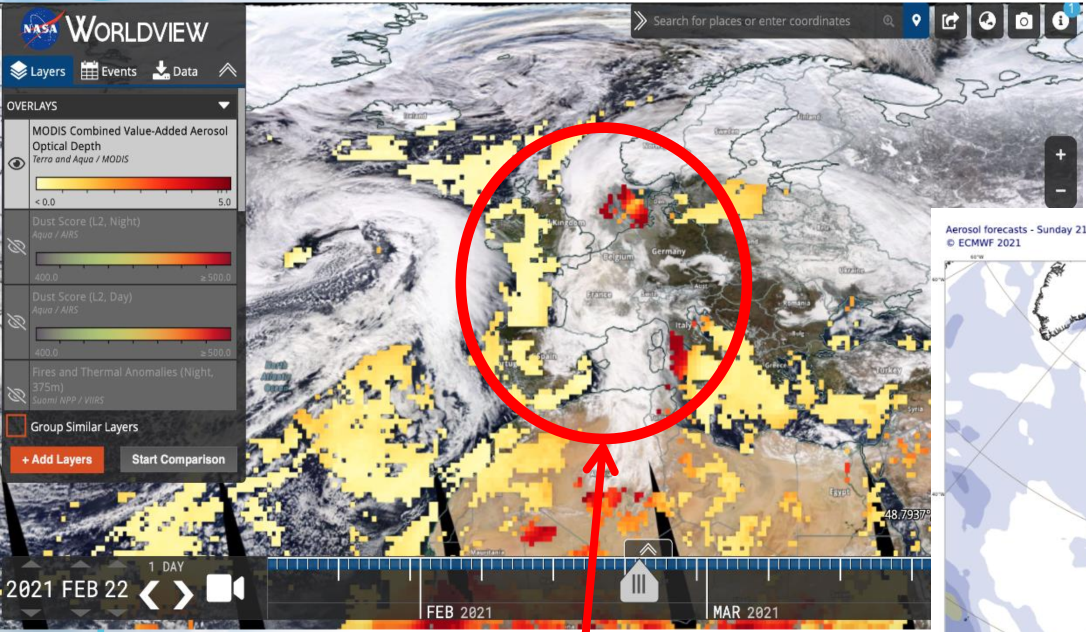




Credit: Nasa Worldview

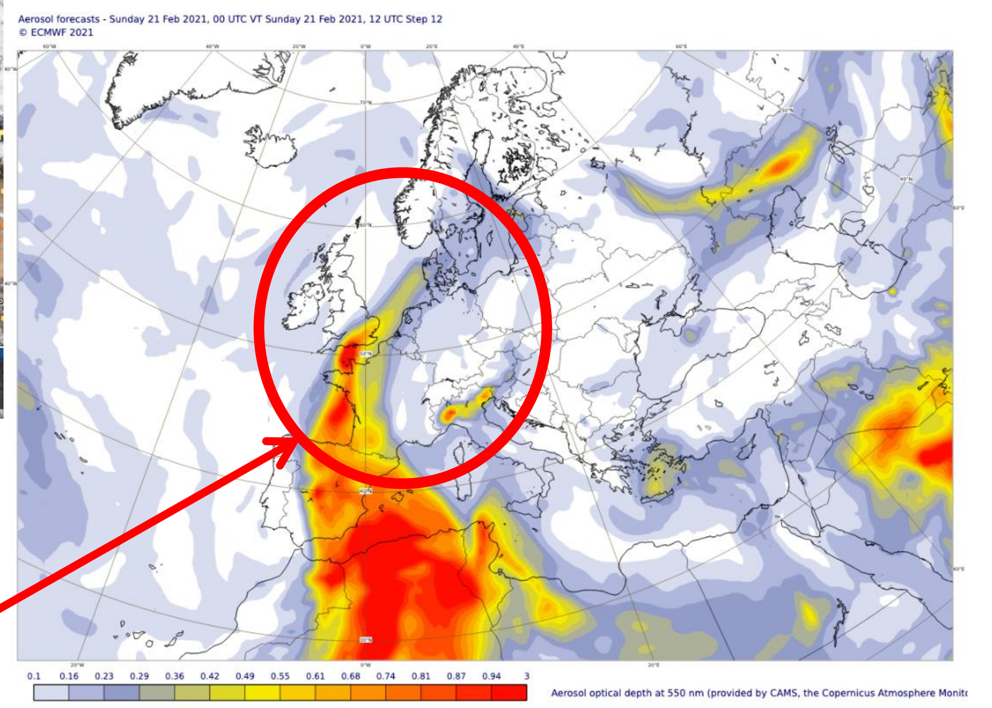
- Assimilated observations are AOD at 550 nm from MODIS (Aqua and Terra) and VIIRS (SNPP and NOAA20) over land and ocean & PMAp (Metop-BC) over ocean
- Control variable is formulated in terms of the **total aerosol mixing ratio**.
- Analysis increments are repartitioned into the species according to their fractional contribution to the total aerosol mixing ratio.
- The repartitioning of the total aerosol mixing ratio increment into the different bins is difficult

Dust storm February 2021



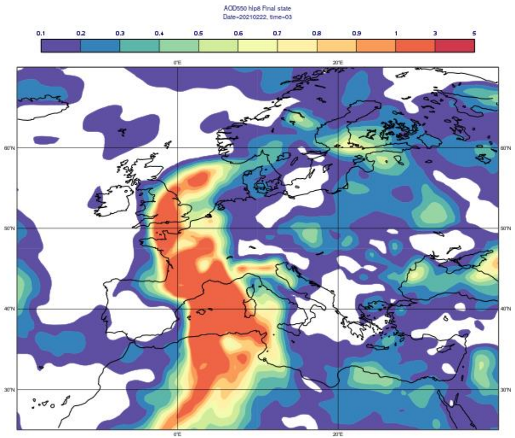
NASA Worldview – MODIS Aqua and Terra AOD 550nm observations for 20210222

CAMS Total AOD at 550nm 12hr forecast valid at 20210222 12hr



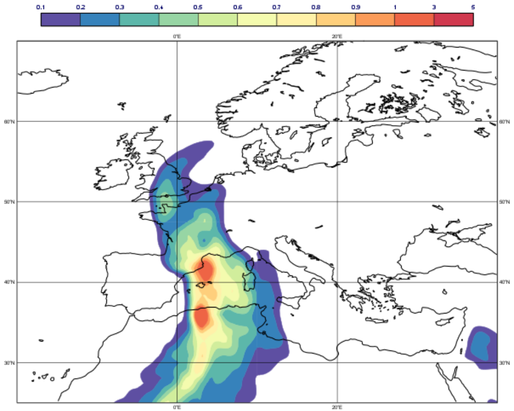
The CAMS forecast does a good job of forecasting the AOD plume from Africa over Northern Europe

Dust test case February 2021

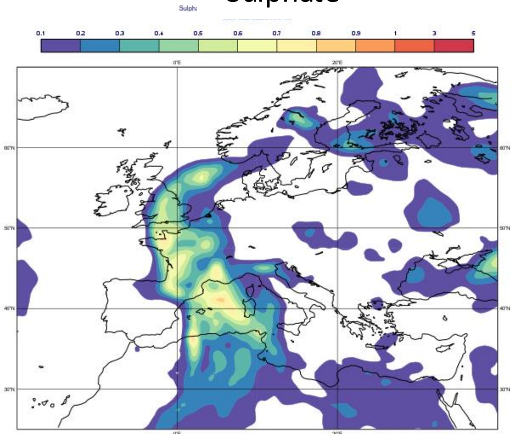


Total AOD at 550nm: 20210222 03hr

Dust

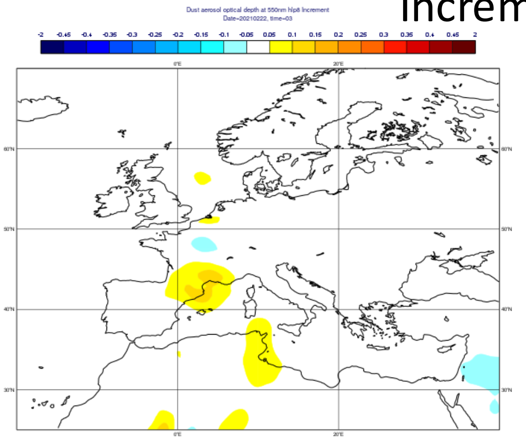


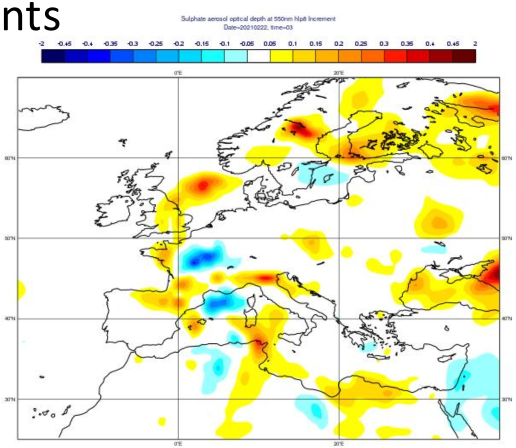
Sulphate



AOD at 550nm

Increments



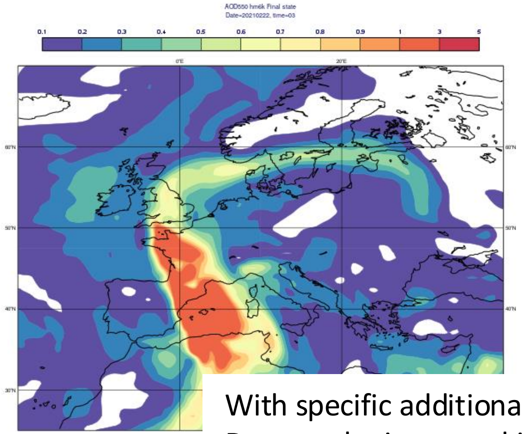


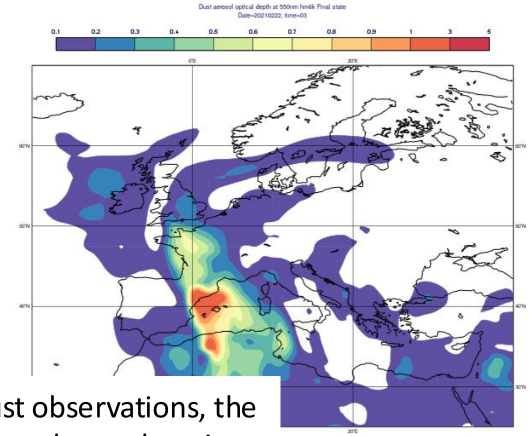
AOD incr at 550nm

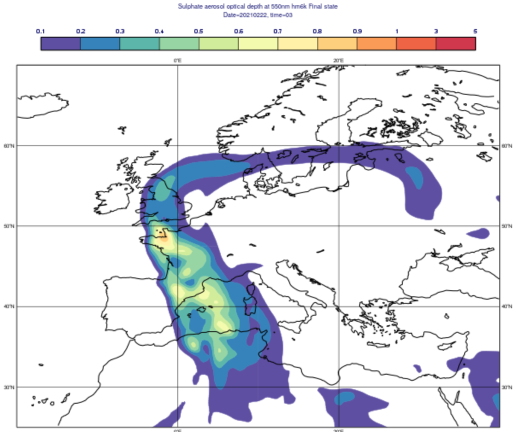
- AOD increments are attributed to the different species according to their proportion in the nonlinear forecast.
- If there is no dust in the forecast in a specific location, then the increment will be given to whatever species are there – in this case Sulphate

European Commission

Dust test case February 2021

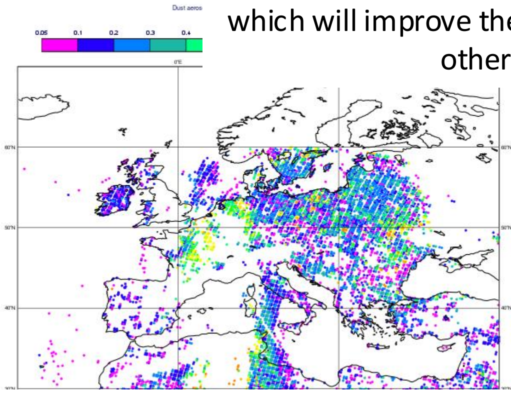




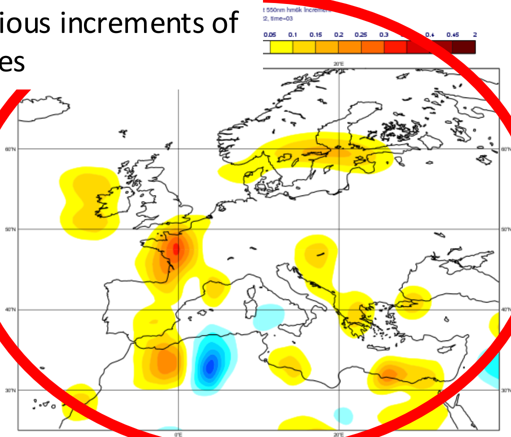


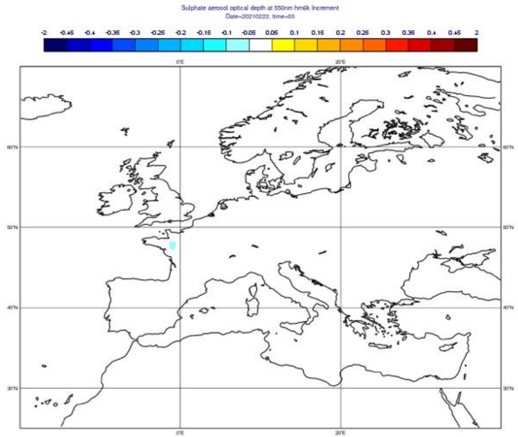
AOD at 550nm

With specific additional Dust observations, the Dust can be increased in the relevant locations which will improve the spurious increments of other species



LMD IASI 10um obs 20210222 12hr





AOD incr at 550nm

Atmosphere Monitoring

6. Potential benefits for NWP

Atmosphere Monitoring

Potential benefit for NWP

- Prognostic aerosols, feedback on dynamics via radiation scheme
- Use of O_3 (& other fields) in the radiation scheme
- RTTOV observation operator: Use of O_3, CO_2 analysis fields to improve the use of radiances sensitive to O_3, CO_2
- Dynamical coupling with wind/T through TL and AD
- Multivariate JB: Correlations between tracers and dynamical variables, e.g. O_3 and vorticity; correlations between chemical species

Atmosphere Monitoring

Potential benefit for NWP

- **Prognostic aerosols, feedback on dynamics via radiation scheme**
- Use of O3 (& other fields) in the radiation scheme
- RTTOV observation operator: Use of O3, CO2 analysis fields to improve the use of radiances sensitive to O3, CO2
- **Dynamical coupling with wind/T through TL and AD**
- Multivariate JB: Correlations between tracers and dynamical variables, e.g. O3 and vorticity; correlations between chemical species

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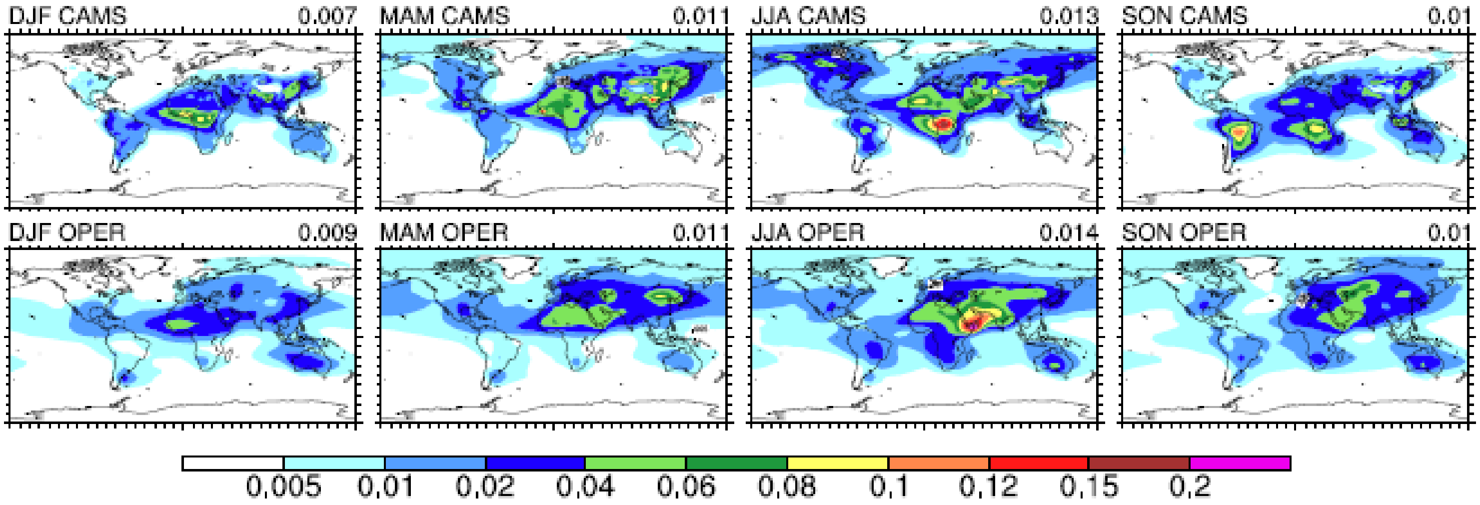
Updated climatology in the radiation

Atmosphere Monitoring

Climatological AOD 550nm distribution CAMS vs Tegen et al 1997

CAMS:

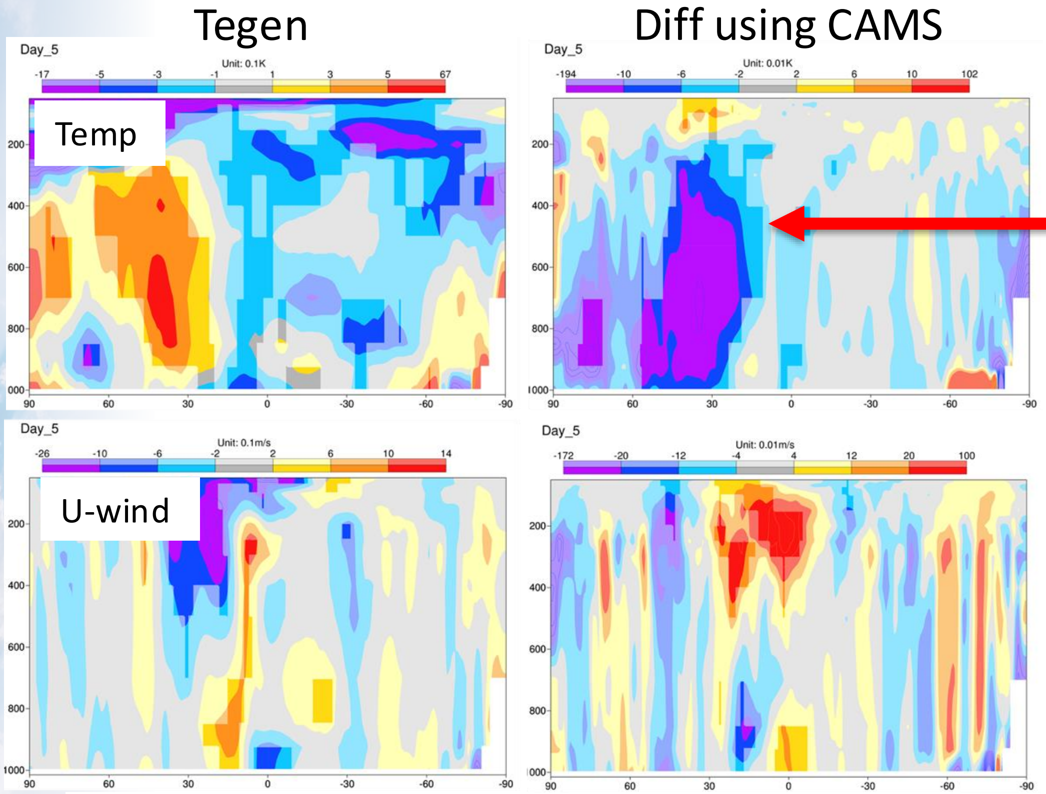
Tegen:



- 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.

Atmosphere Monitoring

Improvements to NWP forecast errors



June-July
Model FC error d+5

June-July
Change in FC error d+5

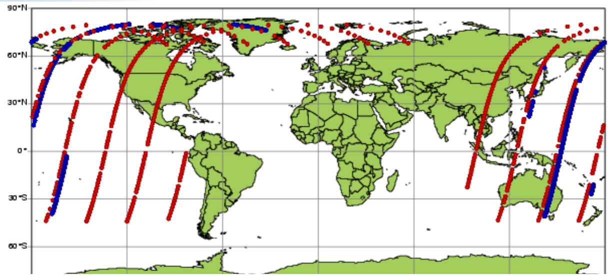
- Change in mass distribution and optical properties -> reduction in SW absorption -> reduction in temperature (positive)
- This is of the order of 0.1K for a bias of the order of 0.3K – it explains at least ~30% of the temperature error.
- Similar for winds at upper levels

Wind information from tracers

Atmosphere Monitoring

- Prospect to extract wind information from long lived tracers in stratosphere and upper troposphere, e.g. O_3, H_2O, N_2O.
- Similar to cloud-track winds but data coverage worse.
- Two ways:
  - Directly through cross correlations between tracer and other variables in background error covariance matrix
  - Indirectly as adjoint of tracer continuity equation propagates the tracer sensitivities over the analysis time window. E.g. O_3 observations can influence the winds indirectly as the system attempts to reduce the O_3 innovations via both wind and O_3 increments
- Potential was demonstrated in early studies for H_2O (Thepaut 1992) and O_3 (Daley 1995; Riishojgaard 1996; Holm 1999; Peuch et al. 2000)
- Could compliment existing wind observations and help in areas where there is a lack of adequate global wind profile data

Example from ERA-Interim (it went wrong)

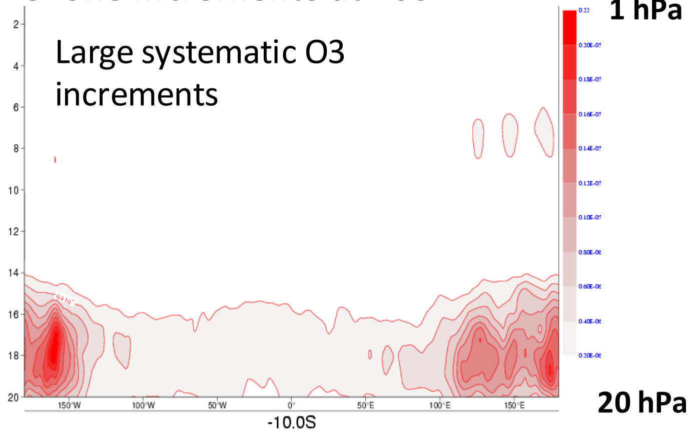


GOME 15-layer profiles (~15,000 per day)
SBUV 6-layer profiles (~1,000 per day)

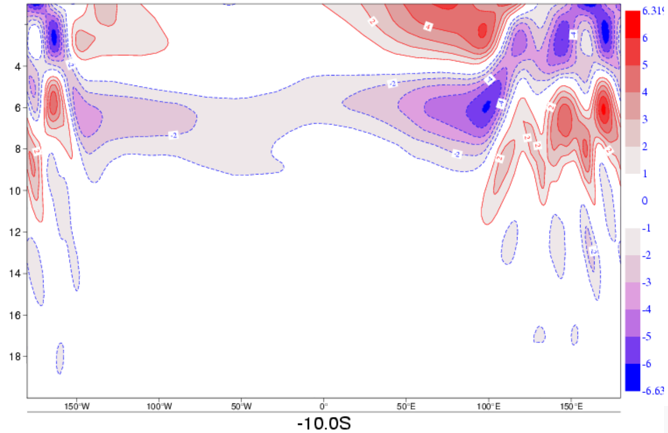
The stratosphere is not well constrained by observations:

- Ozone profile data generate large temperature increments
- 4D-Var adjusts the flow where it is least constrained, to improve the fit to observations

Ozone increments at 10S



Associated Temp increments

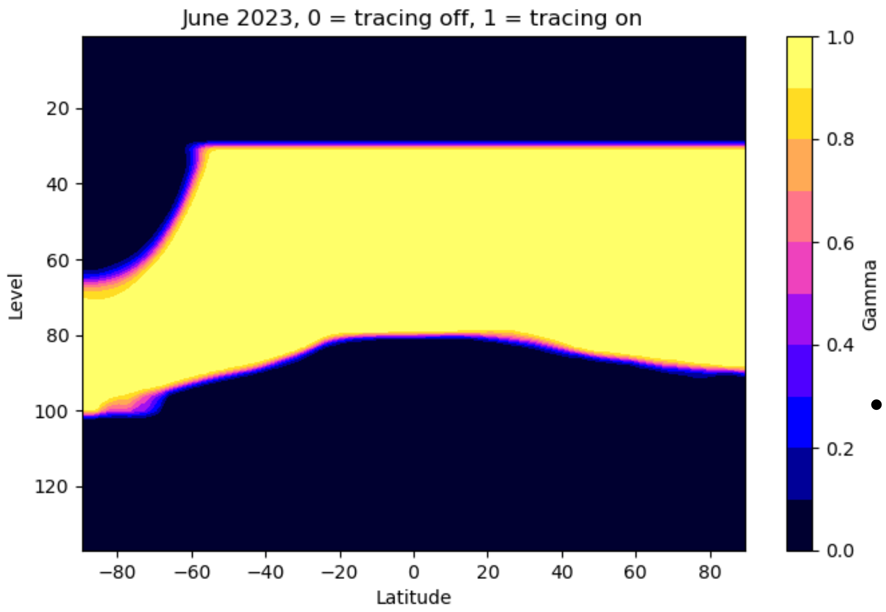


D. Dee

Wind tracing in the next IFS cycle

Atmosphere Monitoring

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



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

- 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
- Flow-dependent γ based on latest background

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

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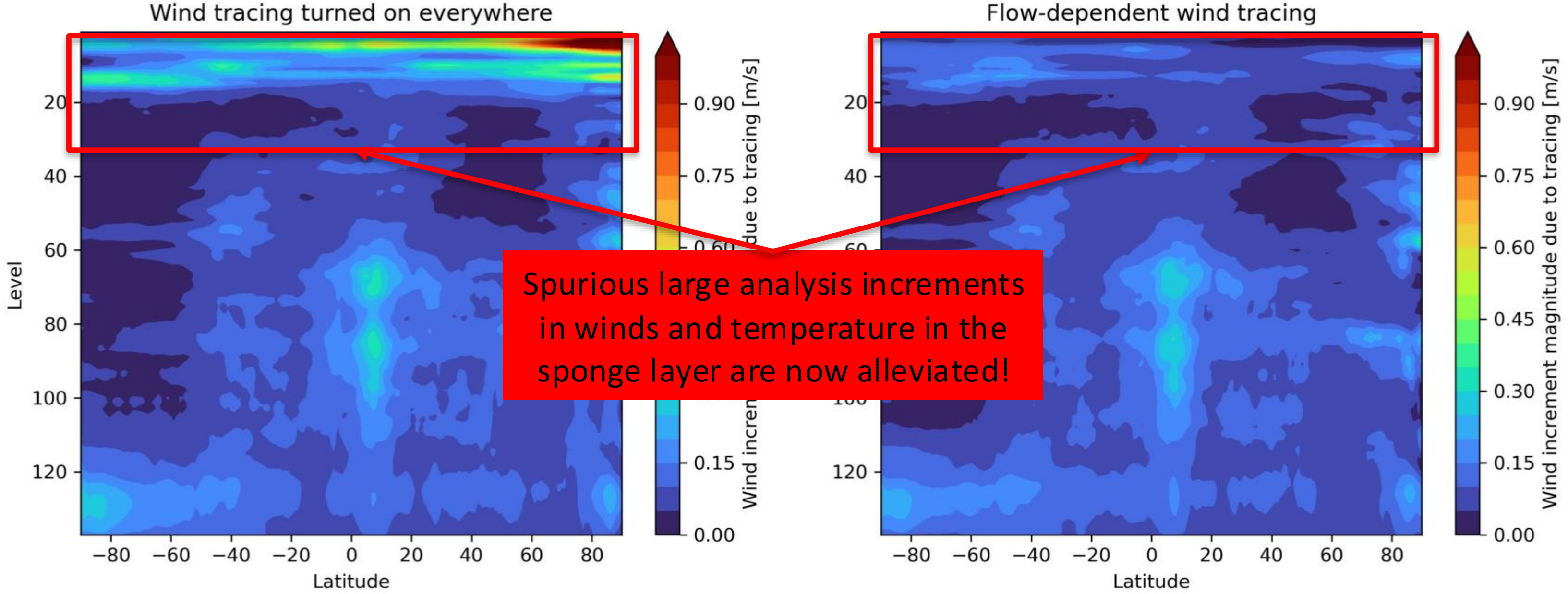
Wind analysis increments



- Positive impact on O-B statistics for ozone-sensitive channels (IASI, CRIS, AIRS), neutral-to-positive impact on other O-B statistics
- Testing synergies between MLS O3 assimilation and ozone-wind tracing

Atmosphere Monitoring

7. Summary

What we have seen today…

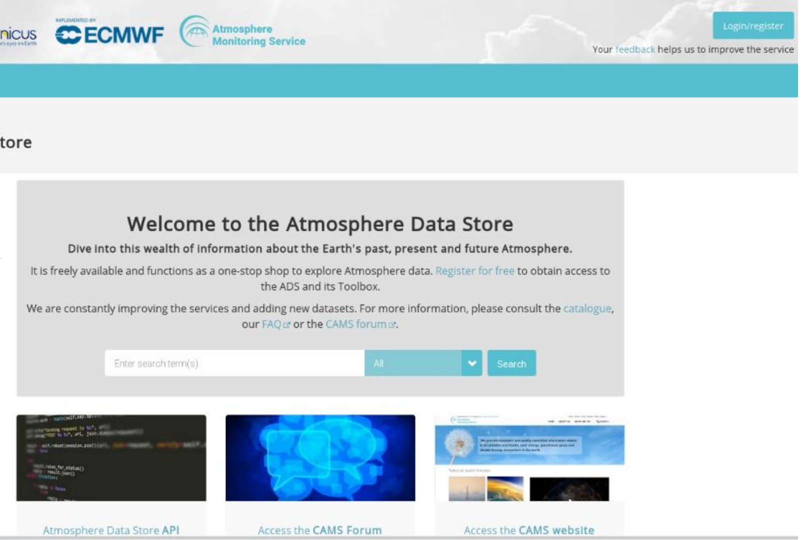
- Basic Data Assimilation theory is the same
- Particular challenges related to DA for atmospheric composition
  - Boundary conditions (emissions) as well as initial conditions; inversions
  - Mismatches between modelled and observed variables
  - Fast reactions and short life-time of some species
  - Cost of using chemical processes in the minimization (i.e., in the TL/AD models)
- Atmospheric composition has the potential to improve various aspects of NWP
- CAMS produces useful global and regional European Atmospheric Composition forecasts and analyses, freely available from **atmosphere.copernicus.eu**

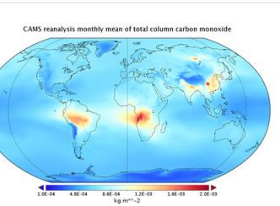
Atmosphere Monitoring

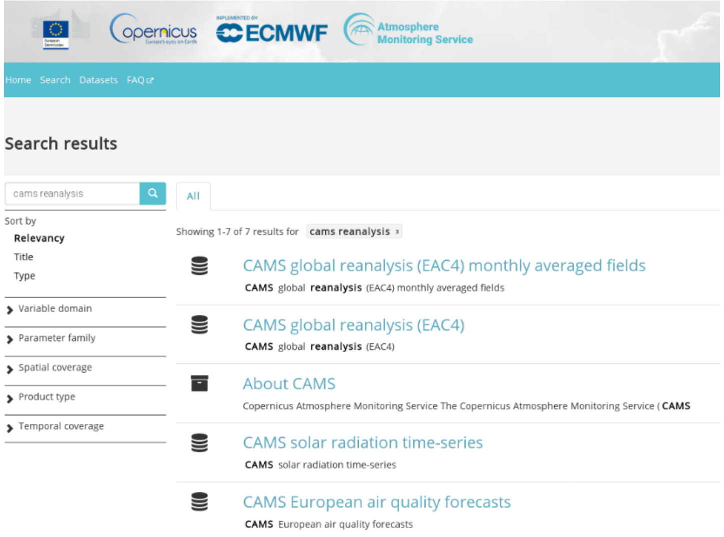
The Atmosphere Data Store (ADS)

All CAMS data are freely available

https://atmosphere.copernicus.eu/data







http://atmosphere.copernicus.eu | @CopernicusECMWF | @CopernicusEU

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References: Reactive gases

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