Data assimilation of atmospheric composition

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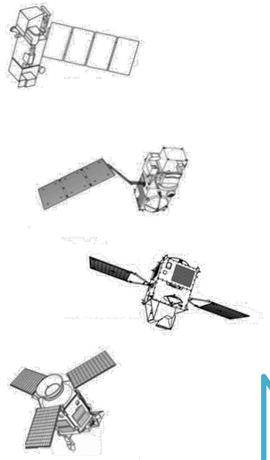
ECMWF

Why atmospheric composition at an operational weather prediction centre?

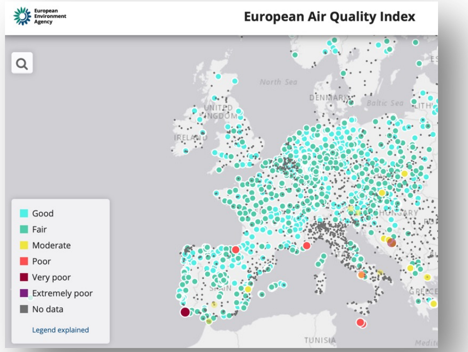
- Poor air quality is a major public health issue in many countries.
- Local authorities need accurate and timely information to implement effective air pollution mitigation measures.
- Accurate air quality forecasts require accurate transport models.
- Can leverage sophisticated data acquisition infrastructures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

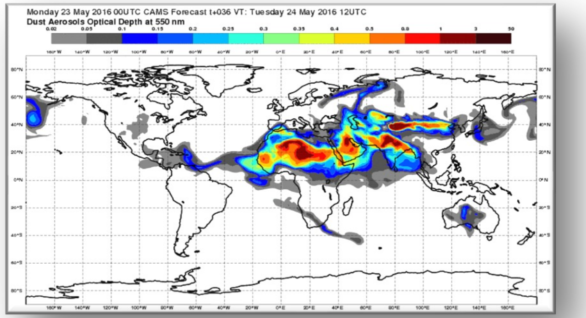
Atmosphere Monitoring Service
atmosphere.copernicus.eu

Copernicus Atmosphere Monitoring Service



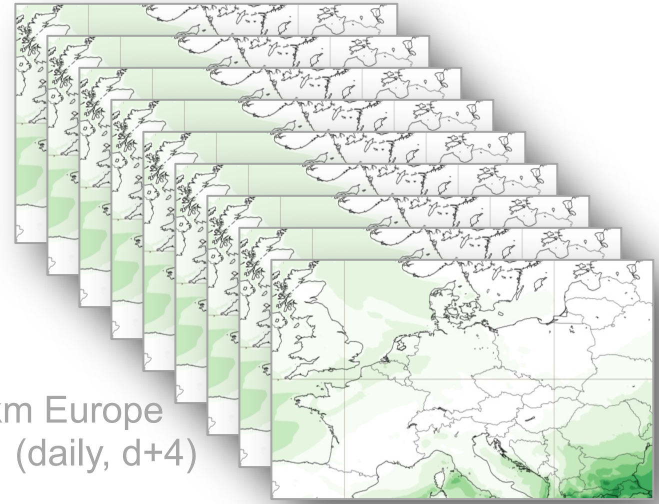
Earth Observation from satellite (>80 instruments) and in-situ (regulatory and research)





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)

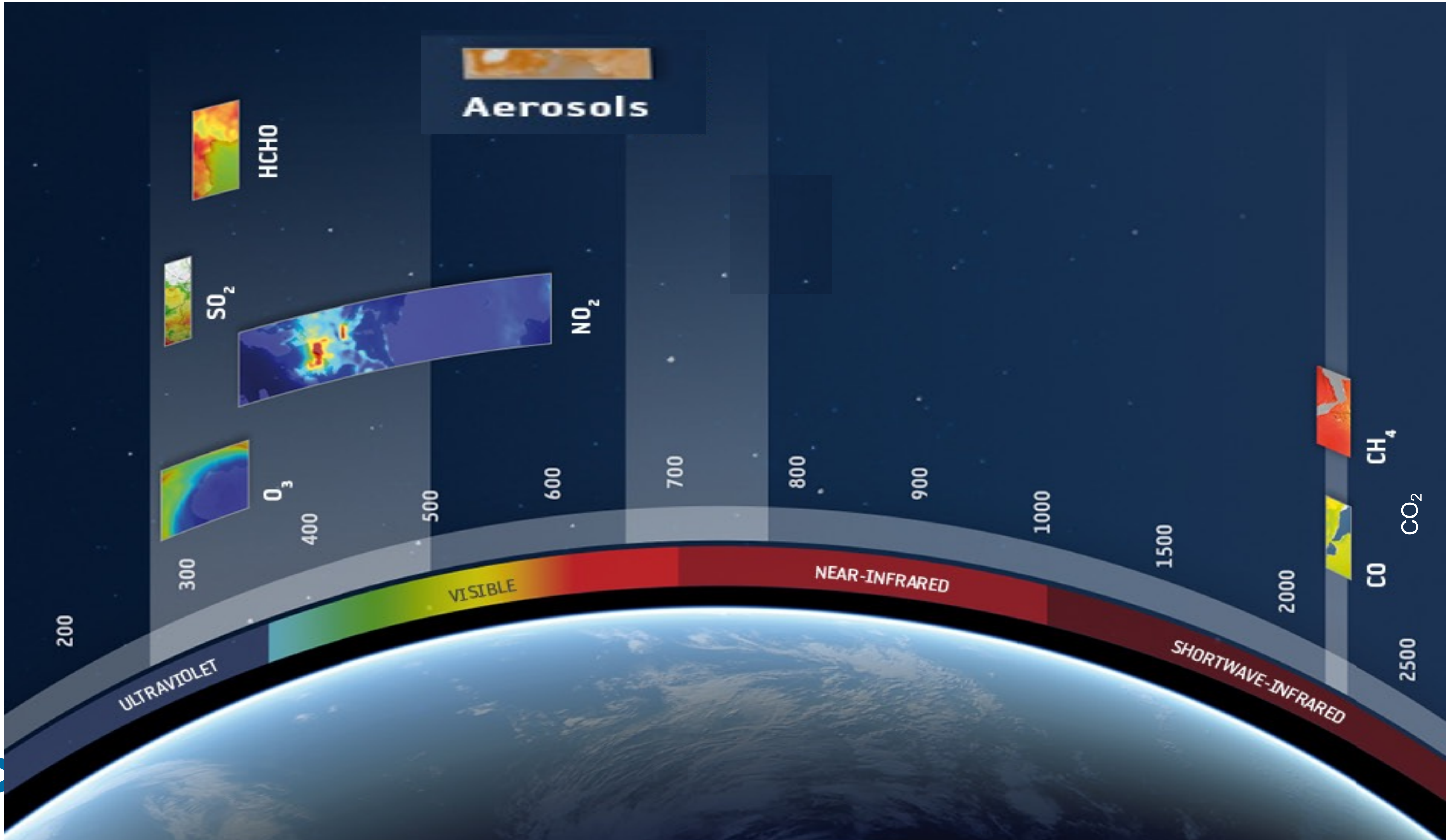
ECMWF
EUROPEAN CENTRE FOR MEDIUM-RANGE WEATHER FORECASTS

What can we actually observe?

Focus on satellite observations for a global forecasting system

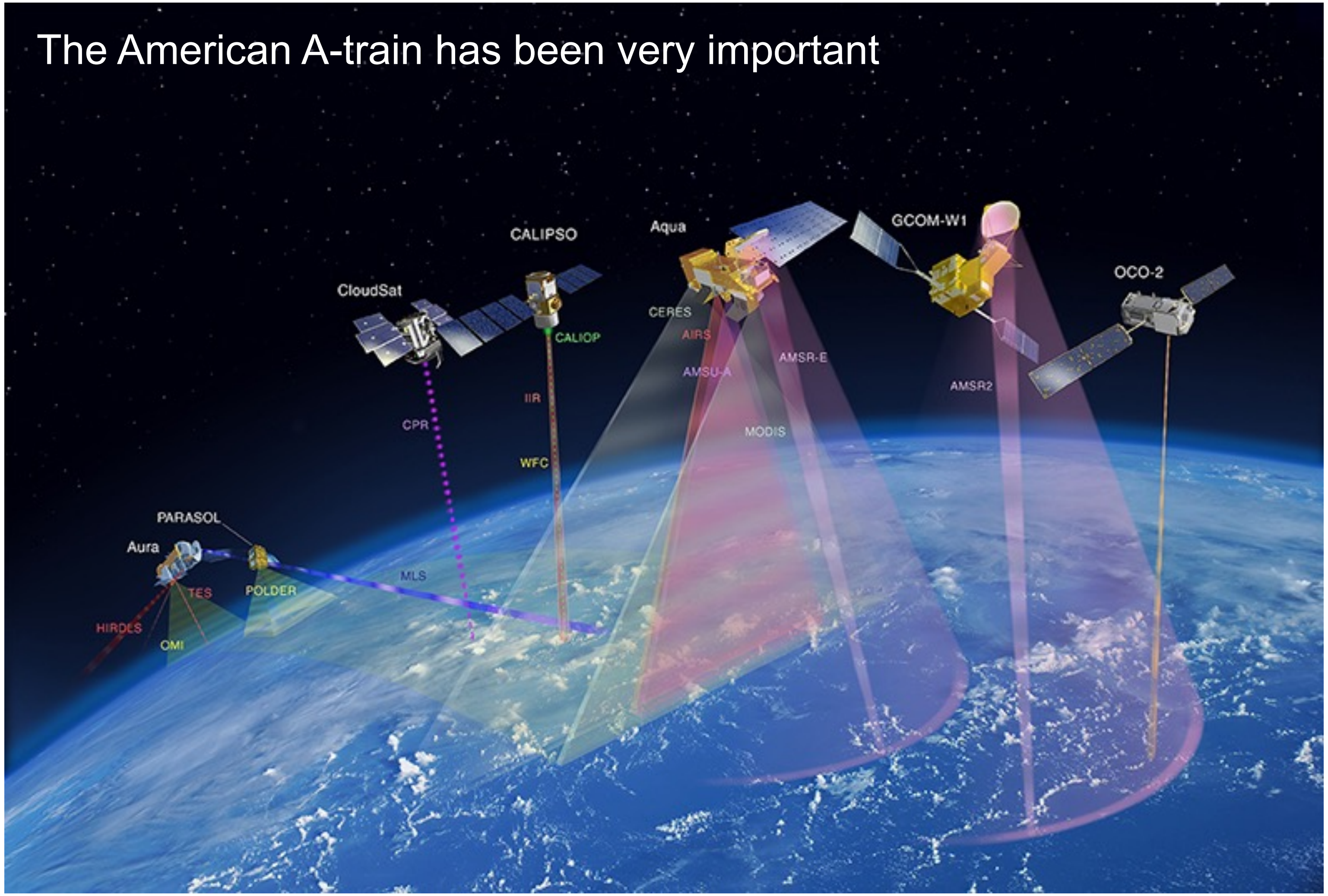
Spectral bands and different species observed

UV to SWIR



Satellite observations

The American A-train has been very important



IASI & GOME-2 onboard the European MetOp satellites have also provided a wealth of atmospheric composition data.

Satellite observations

Satellite data assimilation/integration at ECMWF for CAMS forecasts

	O_3					CO			NO_2		SO_2		AOD				CH_4			CO_2		
Satellite	AURA		Metop BC	S-NPP & NOAA 20	Sentinel 5p	Metop AB	TERRA	Sentinel 5p	Metop BC	Sentinel 5p	Metop BC	Sentinel 5p	AQUA & TERRA	Metop BC	S-NPP & NOAA-20	Sentinel-3	GOSAT	Metop BC	Sentinel 5p	GOSAT	Metop BC	OCO-2
Instrument	MLS	OMI	GOME-2	OMPS	TropOMI	IASI	MOPITT	TropOMI	GOME-2	TropOMI	GOME-2	TropOMI	MODIS	PMAP	VIIRS	SLSTR	TANSO	IASI	TropOMI	TANSO	IASI	OCO-2
Type	Strat Profiles	Total Columns	Total Columns	Layers	Total Columns	Total Columns	Total Columns	Total Columns	Tropospheric Columns	Tropospheric Columns	Tropospheric Columns	Tropospheric Columns	AOD	AOD	AOD	AOD	Total Columns	Total Columns	Total Columns	Total Columns	Total Columns	Total columns

Around 20 different data streams are operationally assimilated or monitored into IFS on top of the meteorological data streams.

Data assimilation methodology for atmospheric composition

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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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

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

Chemical module

GHG module

Aerosol module

Chemical Module **IFS**

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

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Atmospheric Composition models

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

Chemical module

GHG module

Aerosol module

Greenhouse Gas Module **IFS**

CHTESSEL
Photosynthesis & ecosystem respiration model
Diagnoses the gross primary production of CO_2 by plants and release of CO_2 by soil

CH_4 comes from prescribed emissions and climatological loss

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Atmospheric Composition models

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

Chemical module

GHG module

Aerosol module

Aerosol bin scheme

IFS

16 aerosol-related prognostic variables:
Sea-salt, Dust, Black carbon, Organic matter, Sulphate, Ammonium, Nitrate and SOA

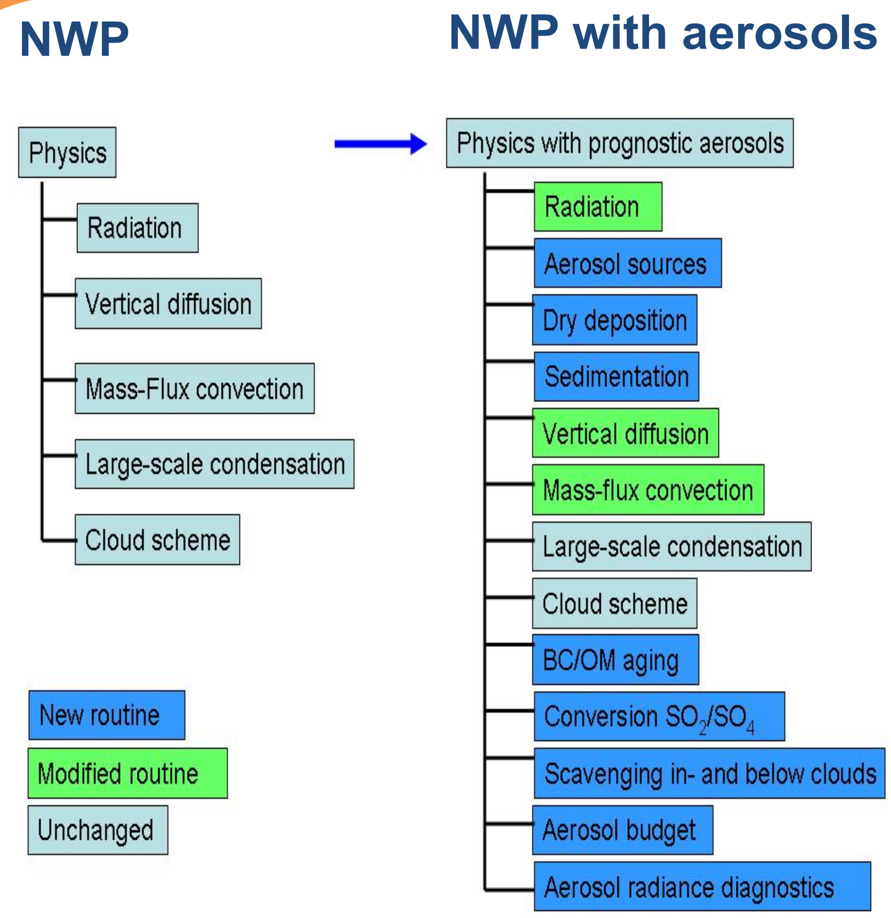
Emissions, dry and wet deposition, sedimentation

Combining the atmospheric composition 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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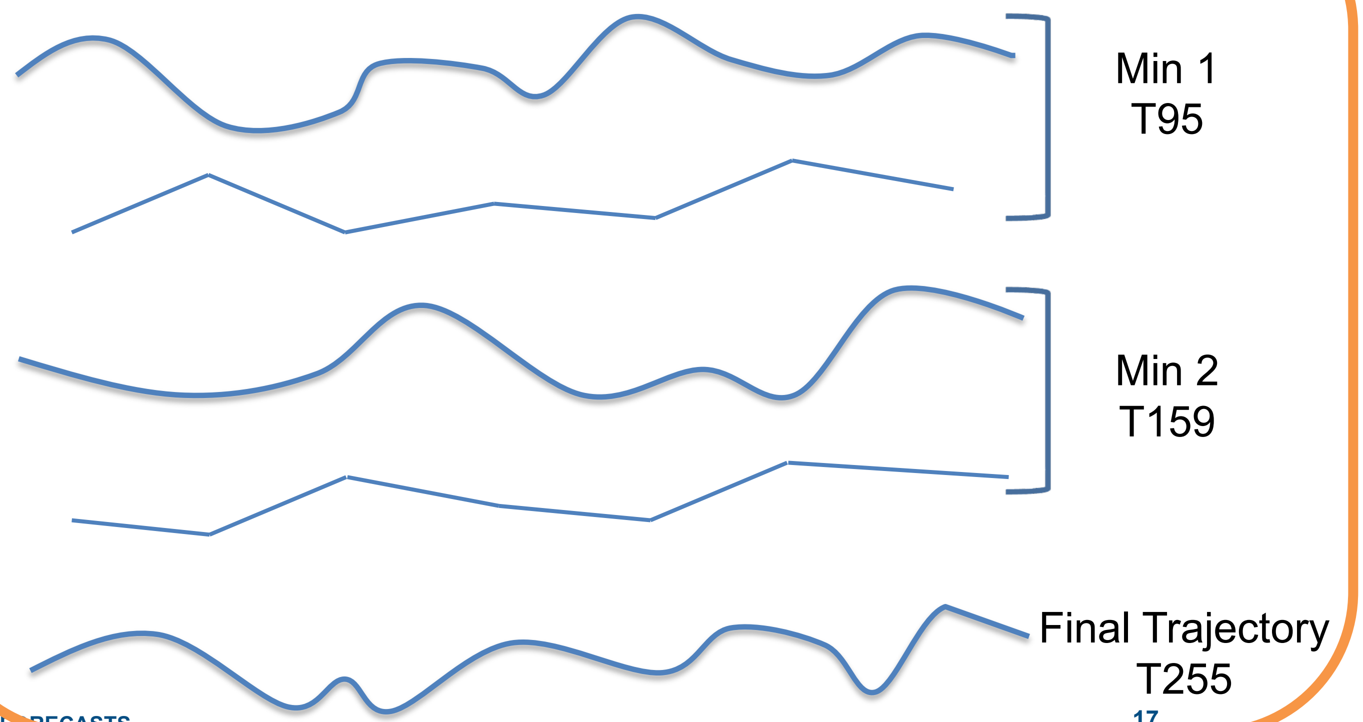
IFS

Data assimilation for the atmospheric composition is 'strongly coupled' (see Coupled Data Assimilation lecture)

Incremental 4DVar



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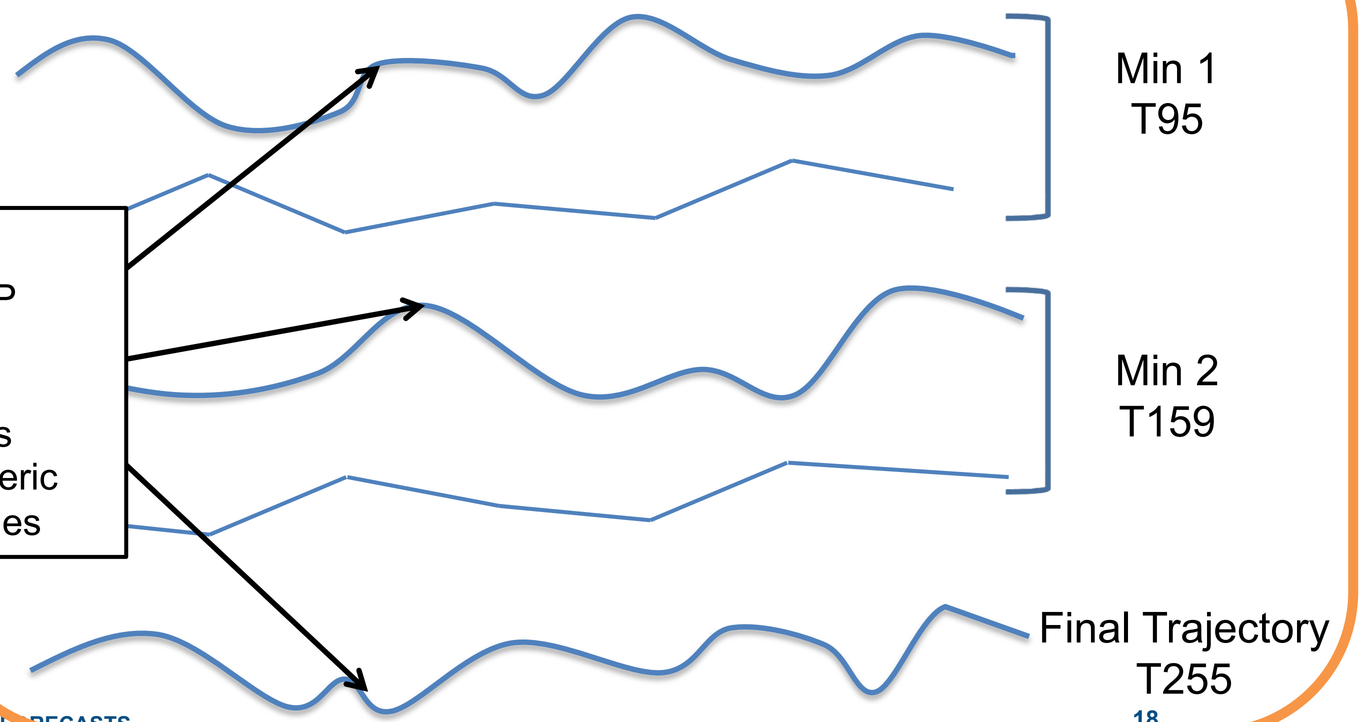
IFS

Data assimilation for the atmospheric compositi ‘strongly coupled’ (see C Data Assimilation lect

Incremental 4DVar

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



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IFS

Data assimilation for the
atmospheric composi
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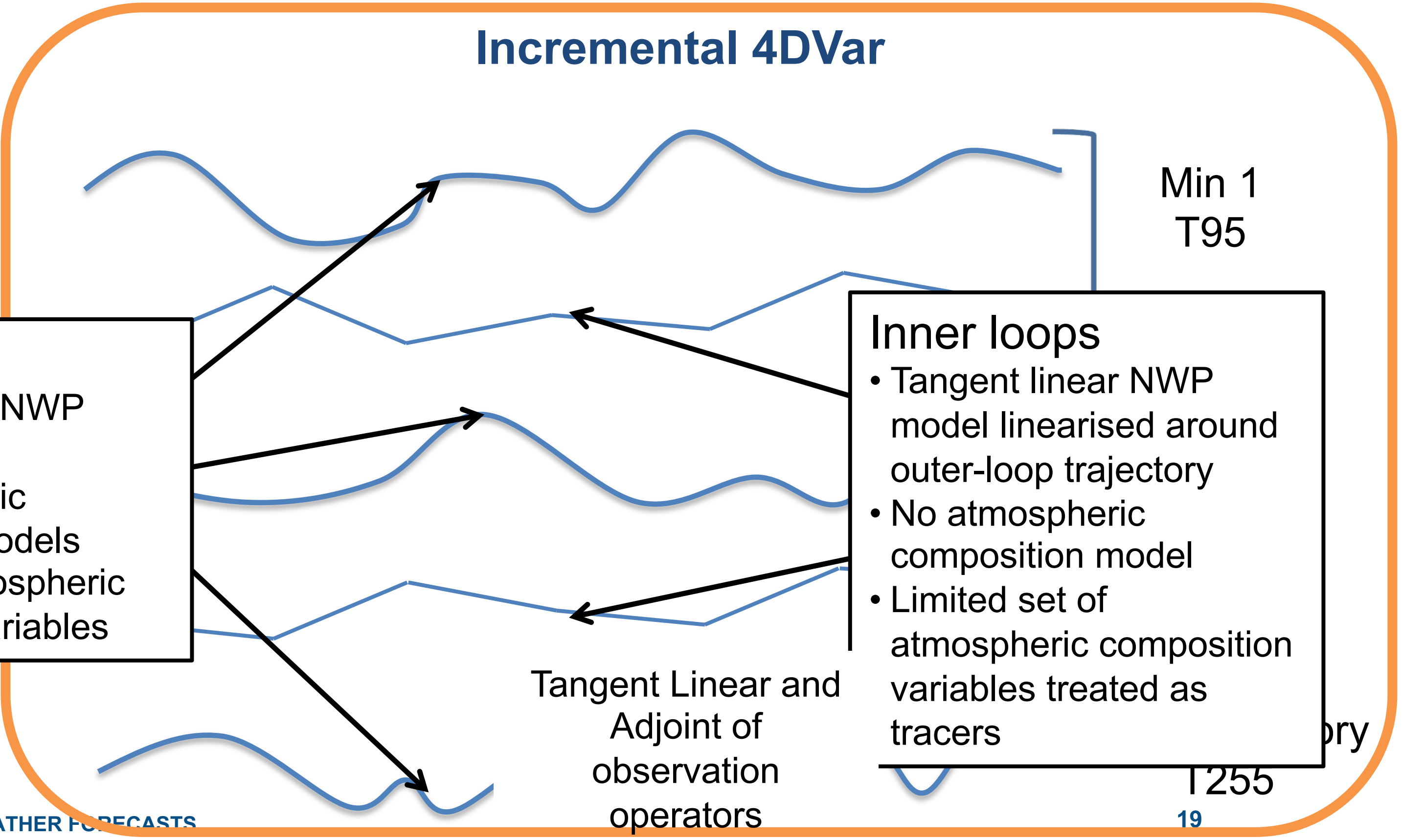
Data Assimilation lect

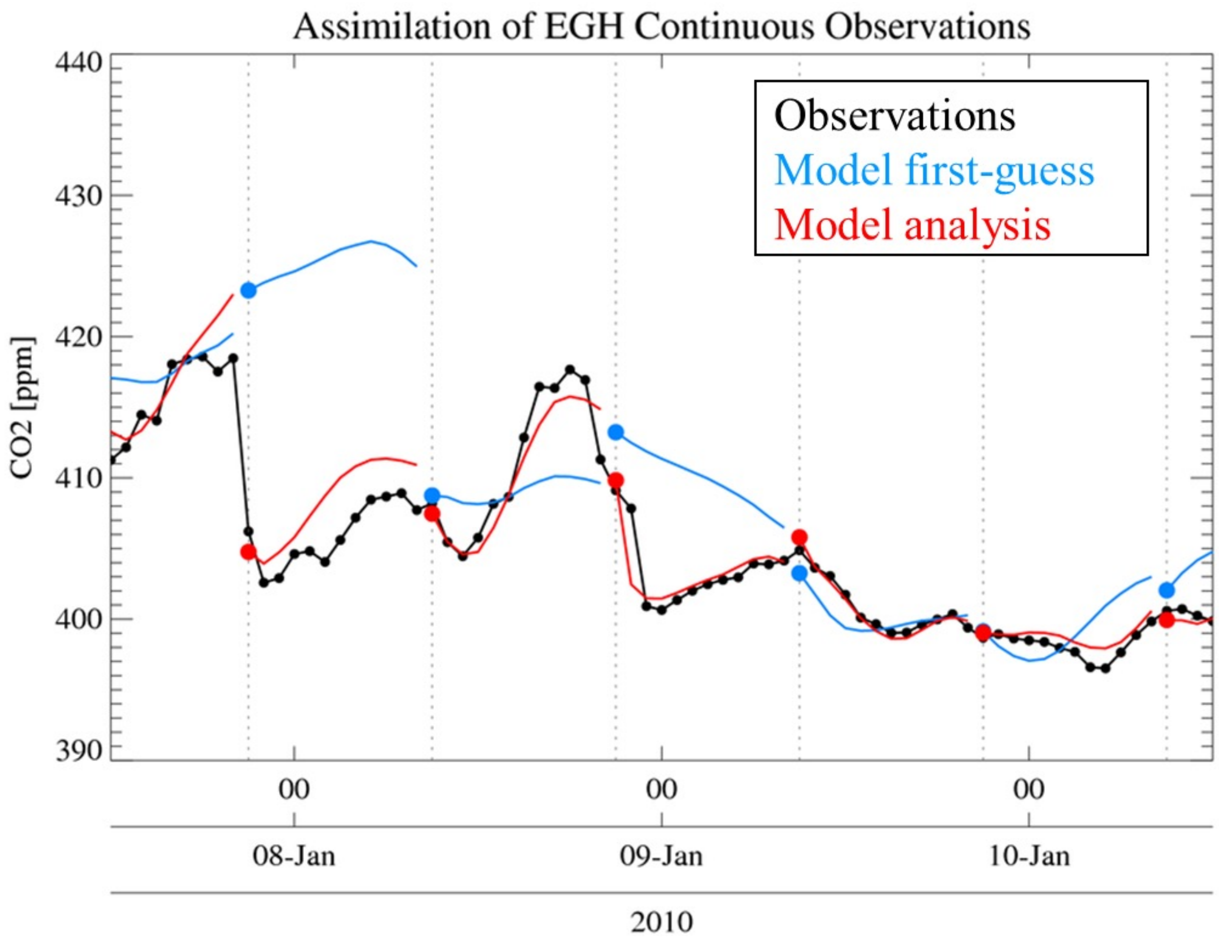


Outer loops
- Full non-linear NWP model
- Full atmospheric composition models
- Full set of atmospheric composition variables

Inner loops
- Tangent linear NWP model linearised around outer-loop trajectory
- No atmospheric composition model
- Limited set of atmospheric composition variables treated as tracers

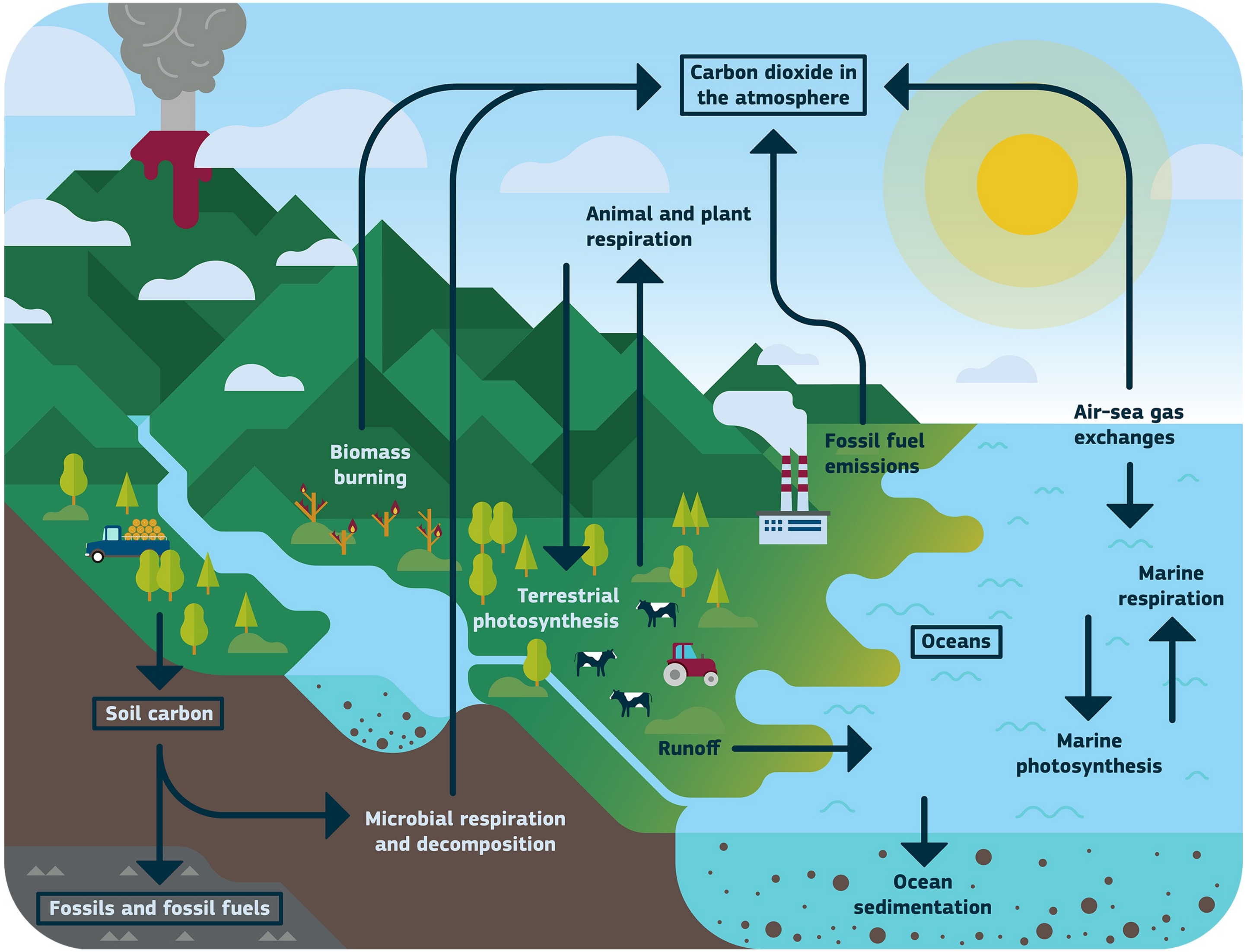
Challenges for Atmospheric Composition Data Assimilation

1. Initial versus Boundary problem



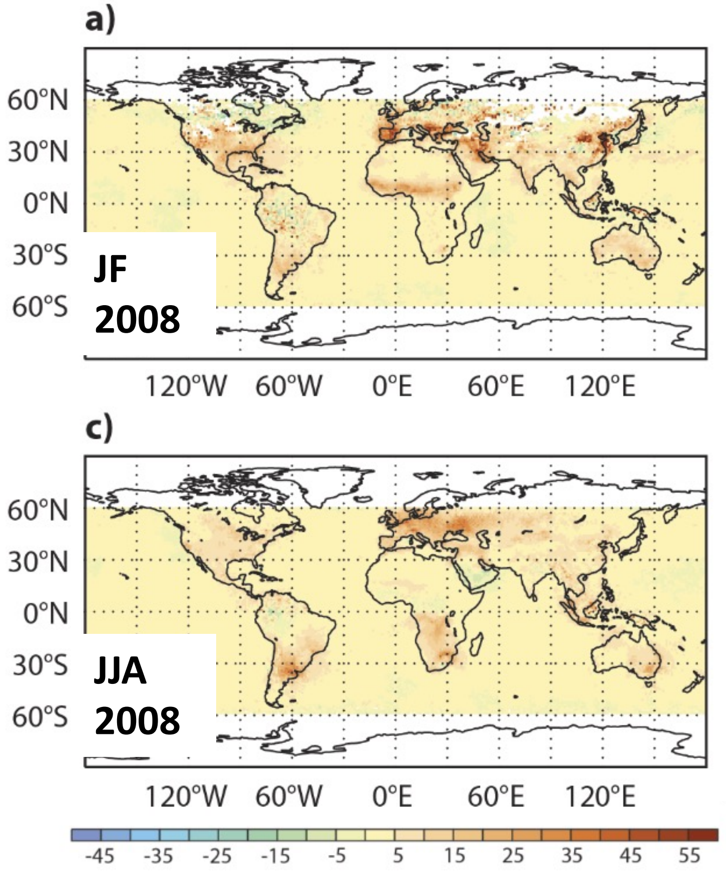
NWP 4D-Var is mostly defined as an initial value problem. Only initial conditions are changed and model error is relatively small.

1. CO_2 as an example – a boundary condition problem

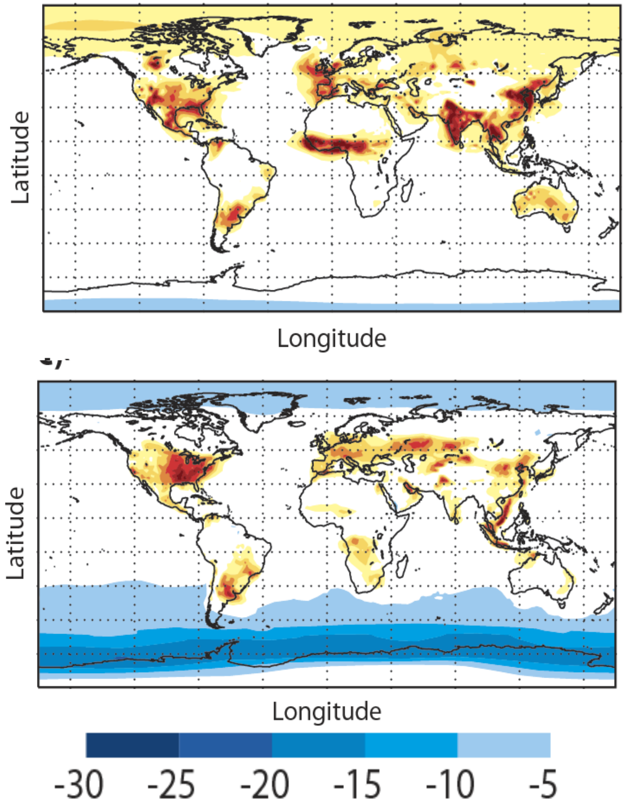


1. Short-lived memory of NO_2 assimilation

OMI NO_2 analysis increment [%]



Differences between Assim and CTRL

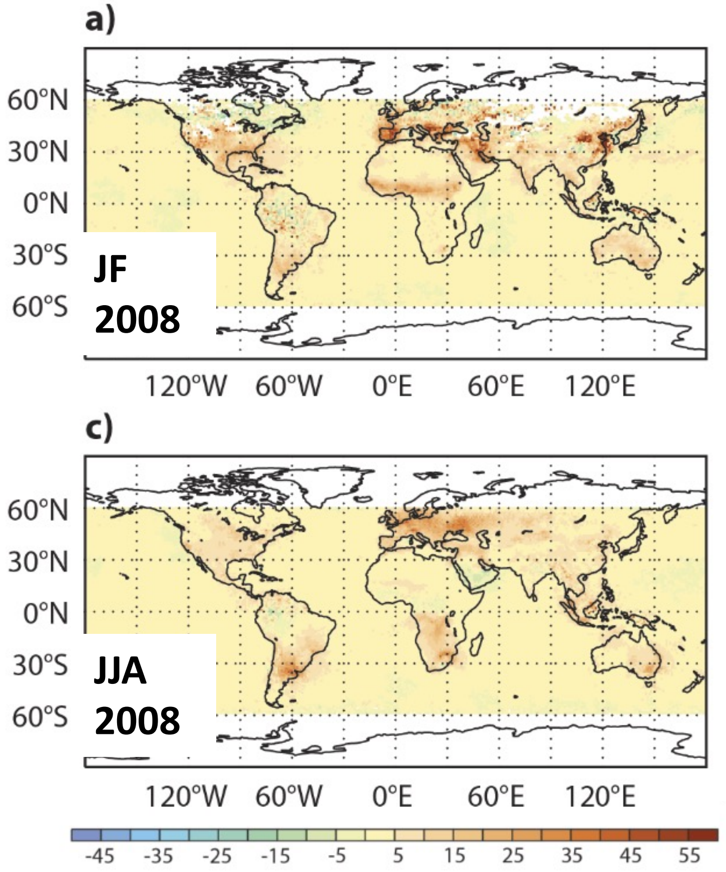


- Large positive increments from OMI NO_2 assim
- Large differences between analyses of ASSIM and CTRL

Inness et al. (2015, ACP)

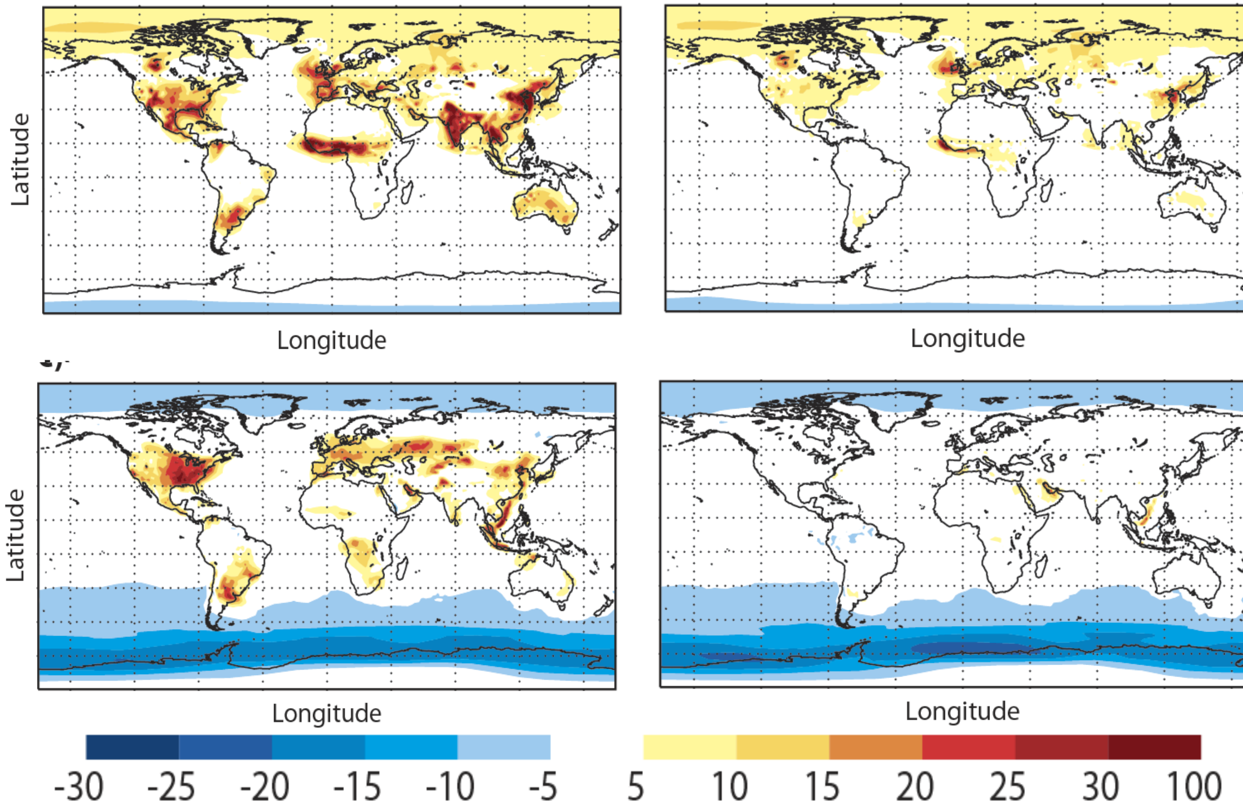
1. Short-lived memory of NO_2 assimilation

OMI NO_2 analysis increment [%]



Differences between Assim and CTRL

Difference between 12h forecasts from ASSIM and CTRL



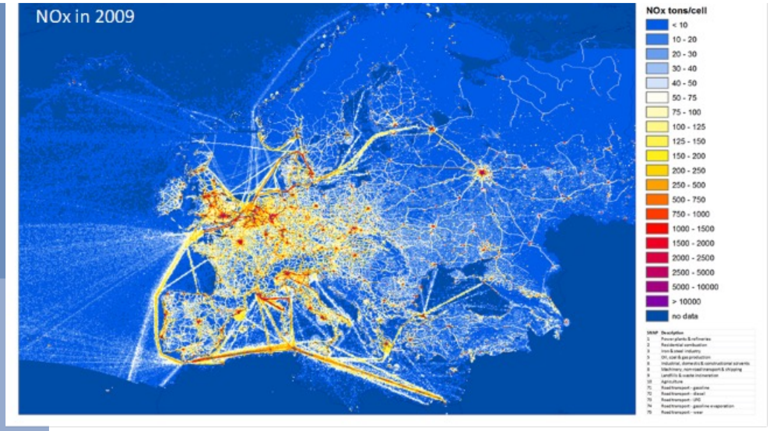
[10^{15} molec/cm²]

- 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

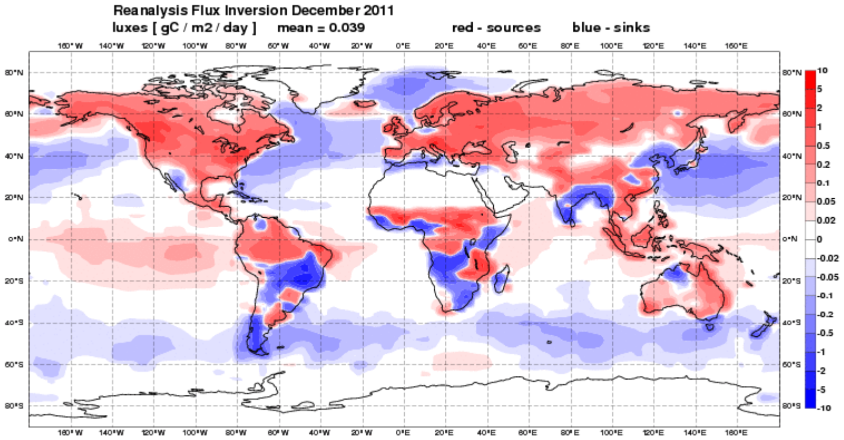
Inness et al. (2015, ACP)

Need for very accurate emission data sets

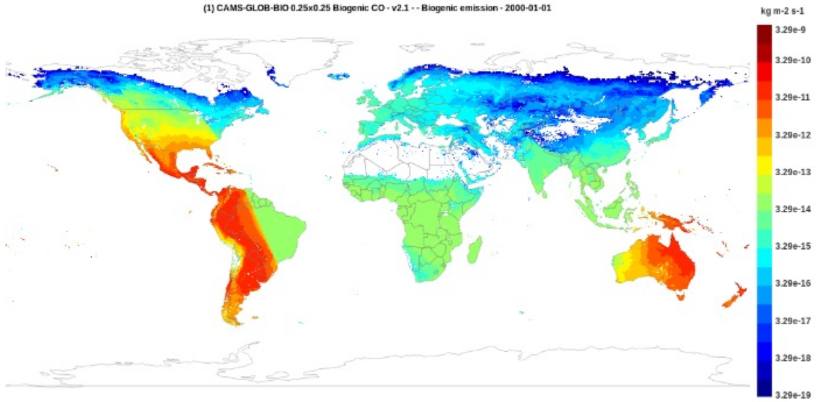
TNO European anthropogenic NOx emissions



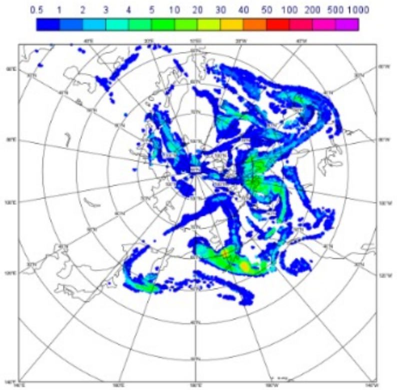
CO_2 fluxes



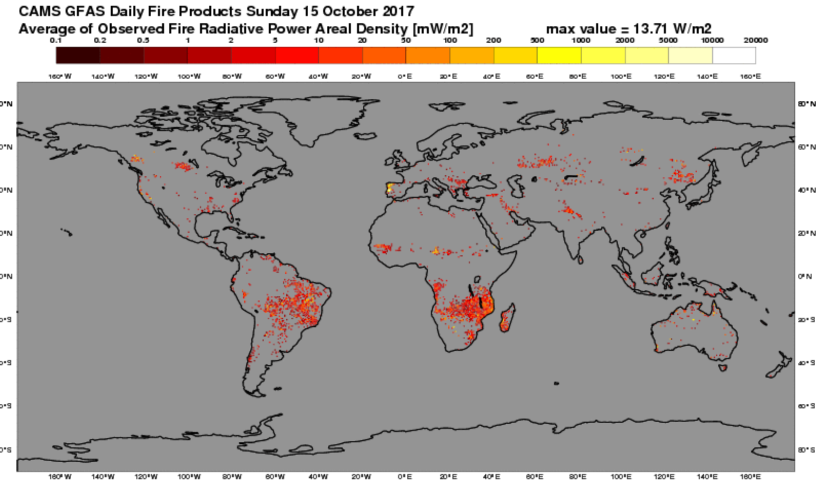
CAMS_GLOB biogenic CO emissions



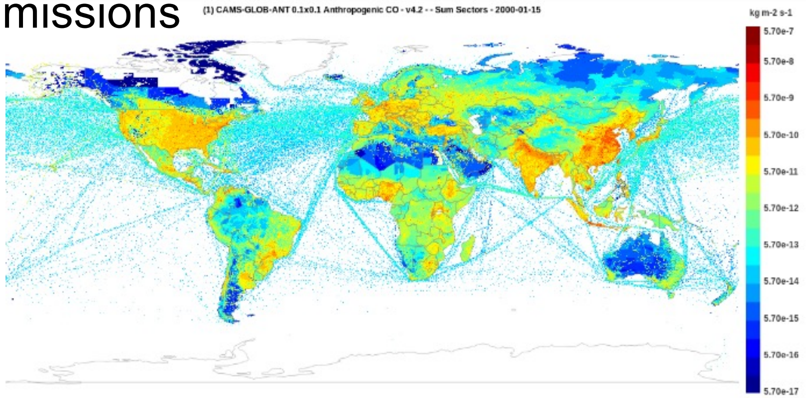
Volcanic SO_2



Biomass burning, 15 October 2017



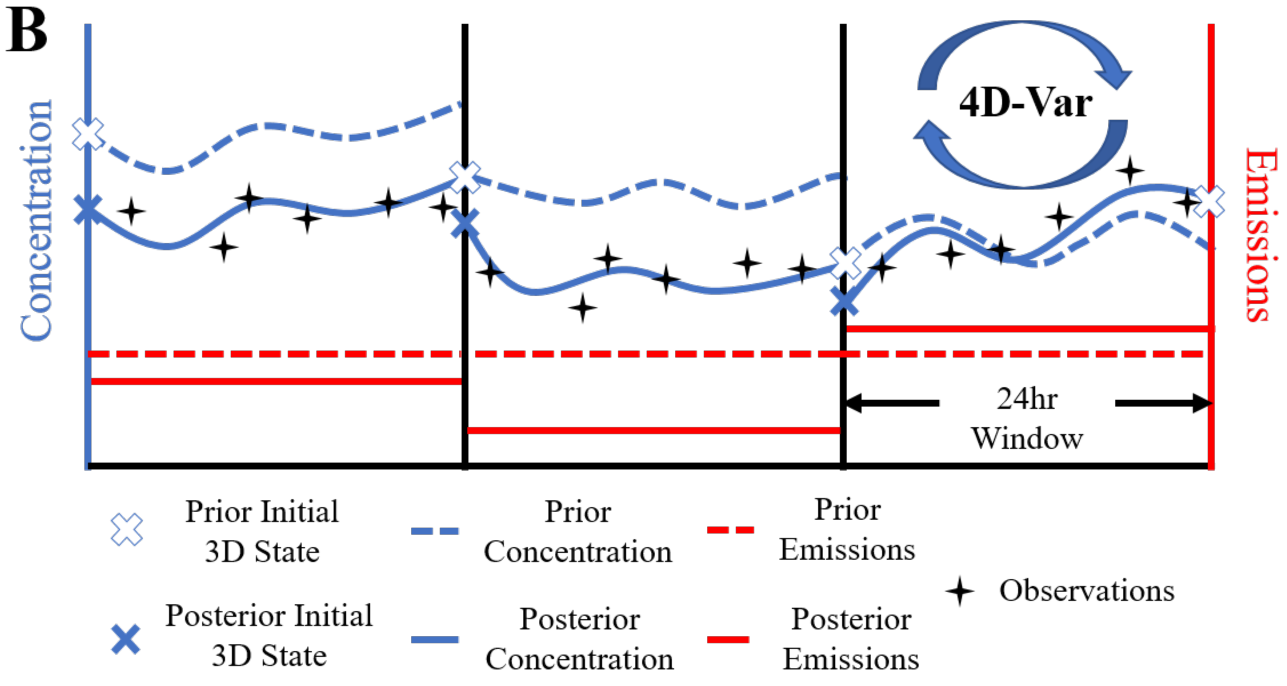
CAMS_GLOB anthropogenic emissions



Emission Estimates

- 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
- 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 emission estimates using observations and models

1. Including emissions in the control vector



McNorton, J., Bousserez, N., Agustí-Panareda, A., Balsamo, G., Engelen, R., Huijnen, V., Inness, A., Kipling, Z., Parrington, M., and Ribas, R.: Quantification of methane emissions from hotspots and during COVID-19 using a global atmospheric inversion, Atmos. Chem. Phys. Discuss. [preprint], https://doi.org/10.5194/acp-2021-1056, in review, 2022.

How to improve?

Use the data assimilation system to adjust surface fluxes at the same time as the initial atmospheric conditions.

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

J_b: background constraint for x

J_p: constraint for emission scaling factors

$$J(x,p) = (x - x_b)^T B^{-1} (x - x_b) + (p - p_b)^T {B_p}^{-1} (p - p_b)$$

State control vector

Parameter (e.g. scaling factors)

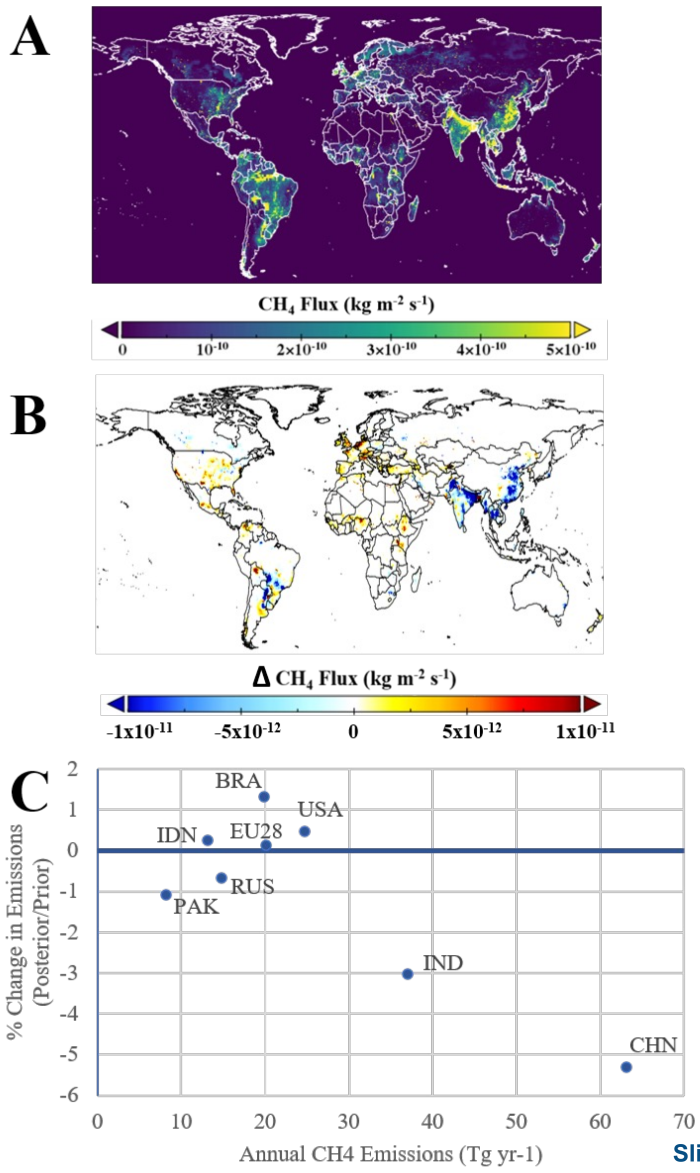
$$+ \sum_{i=0}^{n} (y_i - H_i[x_i, p])^T R_i^{-1} (y_i - H_i[x_i, p])$$

J_o: observation

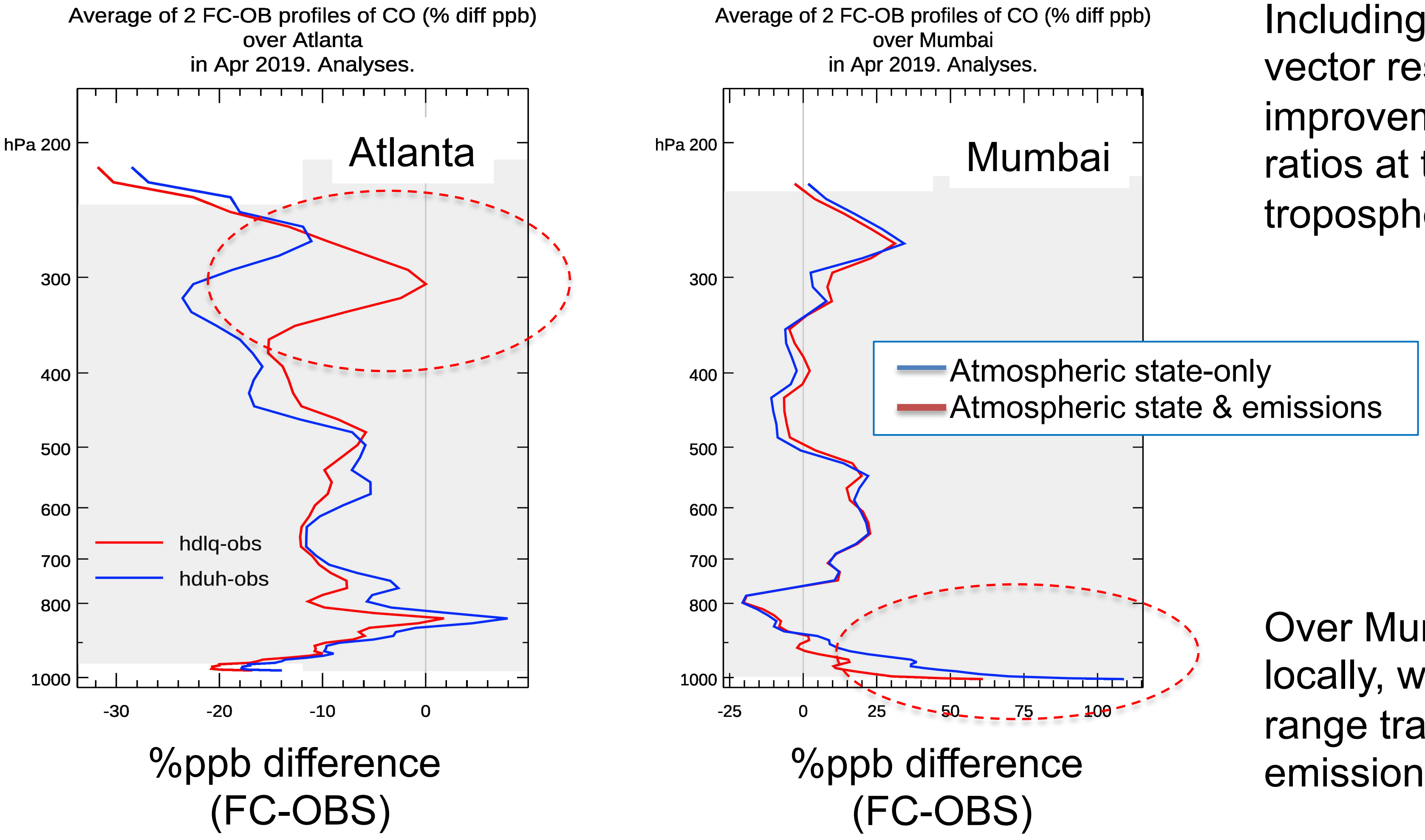
- Joint optimisation of emissions and initial conditions
- Optimized emissions for e.g., CO_2, CH_4, CO, NO & NO_2
- TL/AD of simplified chemistry: link between NO emissions and NO_2 observations
- 2D scaling factors p applied to emission fields
- Prior error definition:
    - Global constant or 2D map 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. Very active research agenda for operational DA for composition

- Include emissions/fluxes in control vector
- Flux increments, correction factor, parameter estimation?
- Enough signal in a typical short assimilation window in operations (6h-12h)?
- How to propagate the information on emission constraints from window to window? No forward model.
- Full chemistry needed (cost)?
- Using co-emitted species for anthropogenic emissions



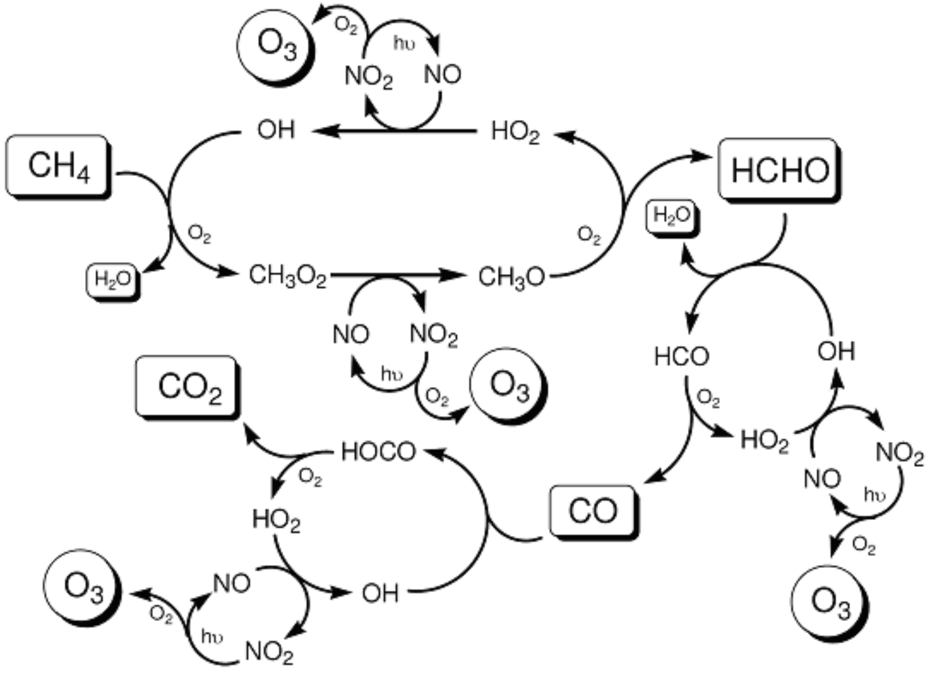
1. Constraining emissions improves the forecast



Including emissions in the DA control vector results in significant improvements in modelled CO mixing ratios at the surface and in the upper troposphere.

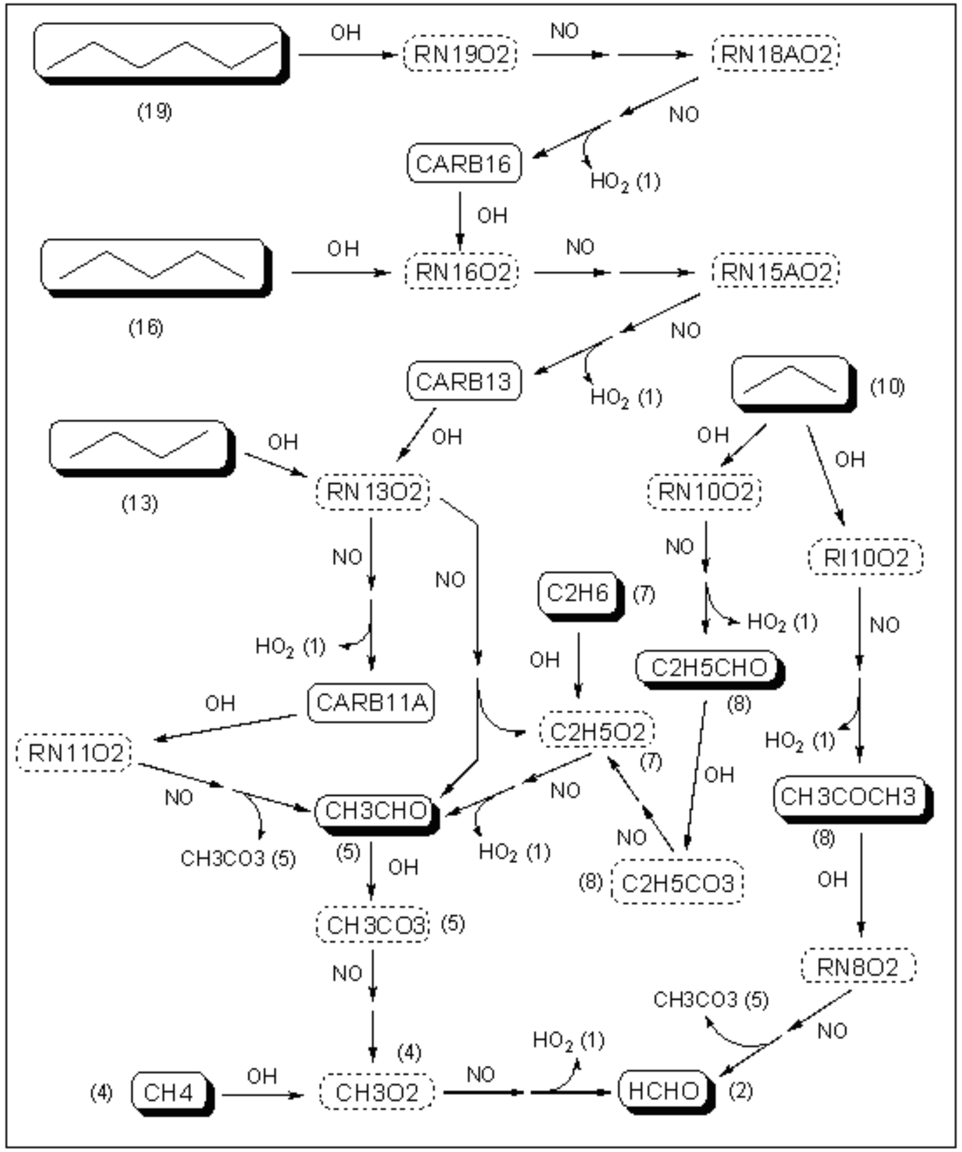
Over Mumbai, emissions are adjusted locally, while Atlanta show the long-range transport effect of adjusted emissions elsewhere.

2. Dealing with many (reactive) atmospheric species

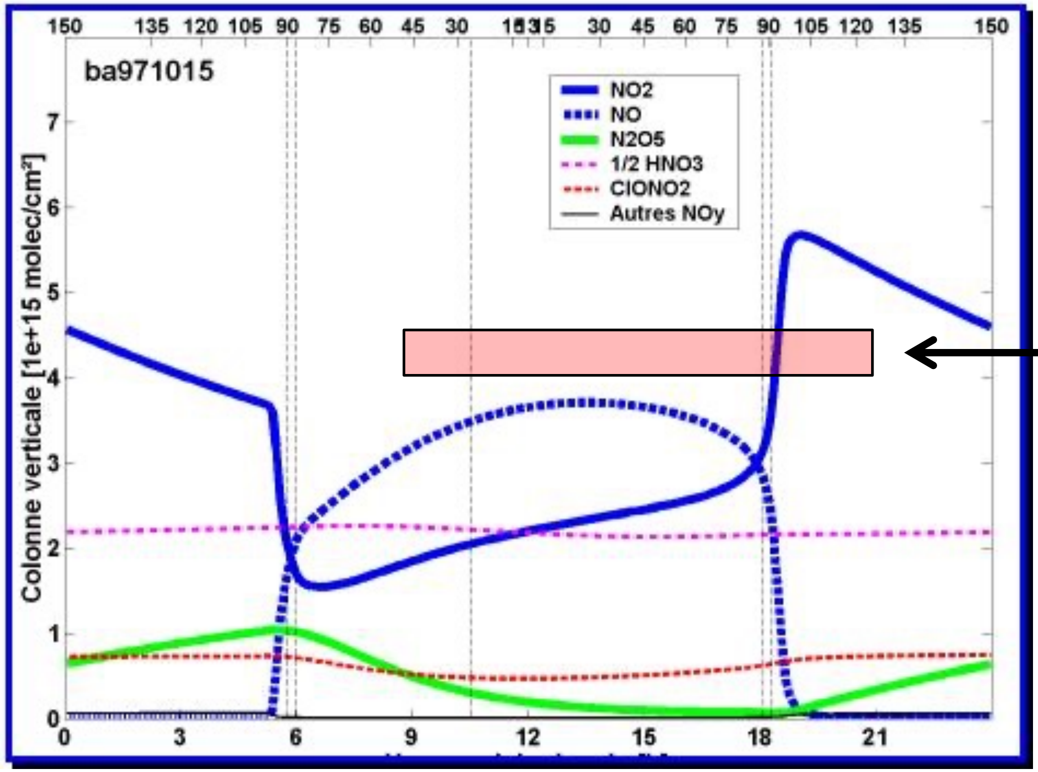


Complexity can go very far… with master mechanisms of about 10000 variables

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

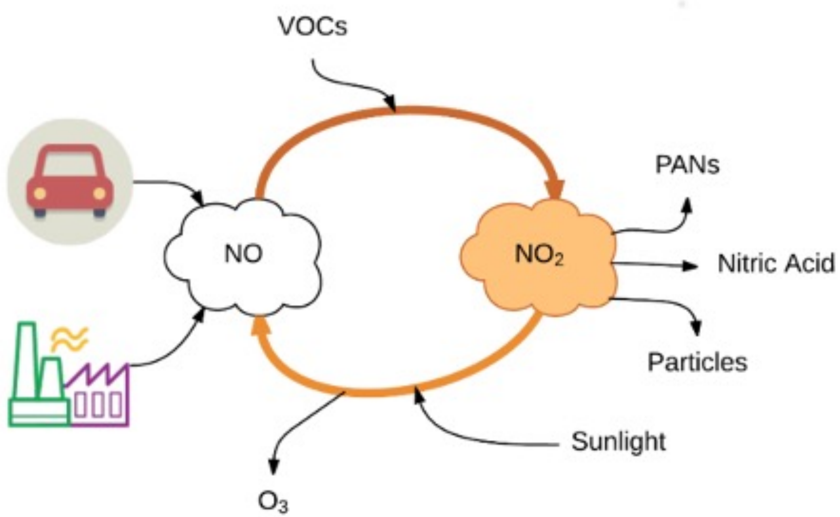


2. Example: assimilating NO_2 satellite observations



12-hour
4D-Var
window

Credits: J-C Lambert (BIRA)



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:

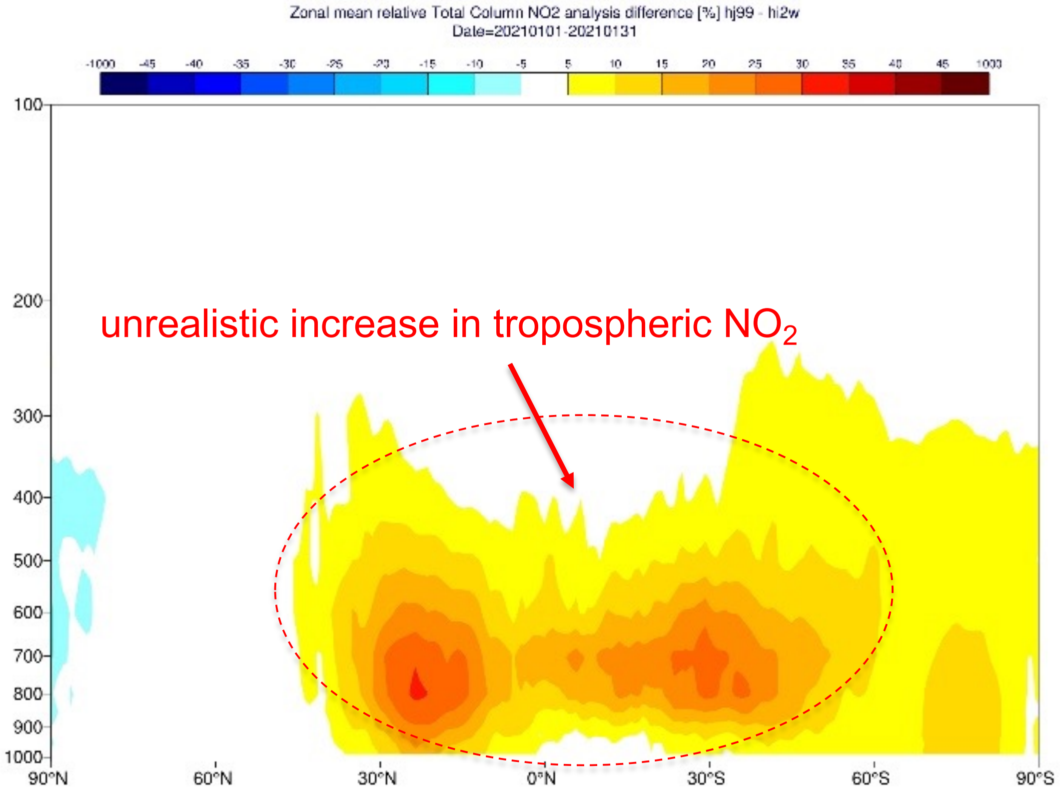
- $NO_2 + OH \rightarrow HNO_3$

> - 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).

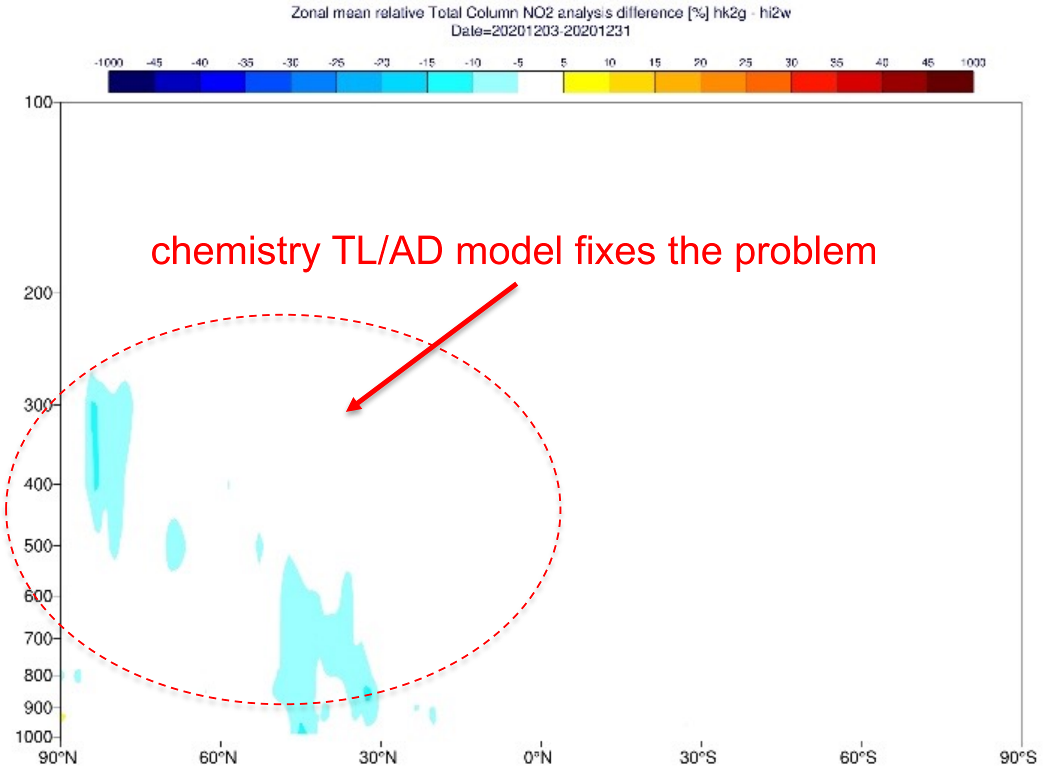
2. Simplified chemistry TL/AD

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

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

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aerosol mixing ratio

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

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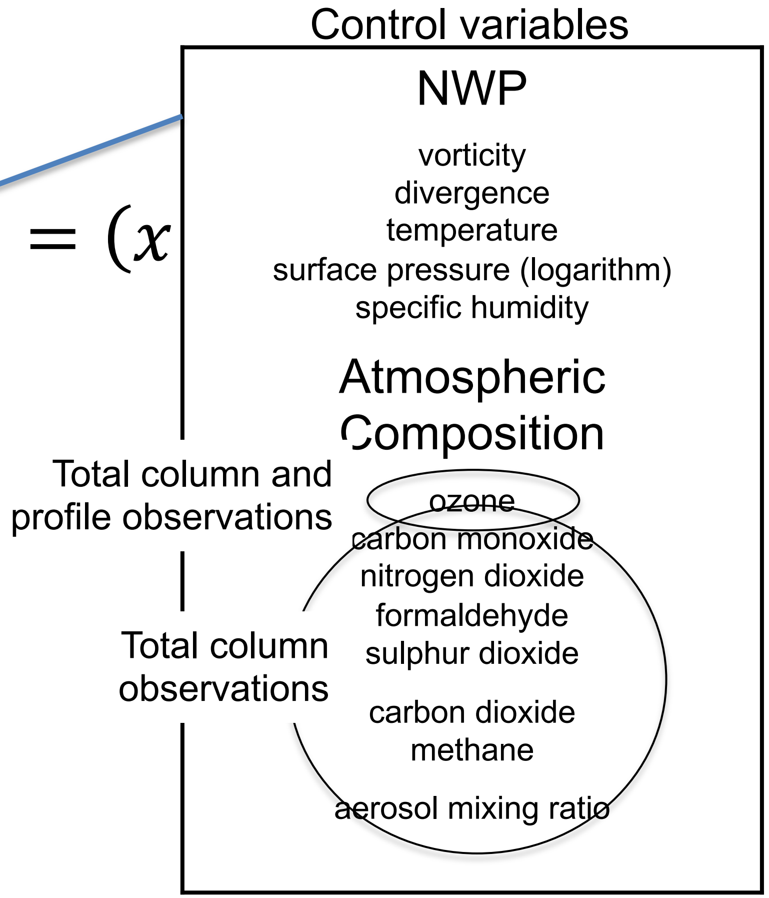
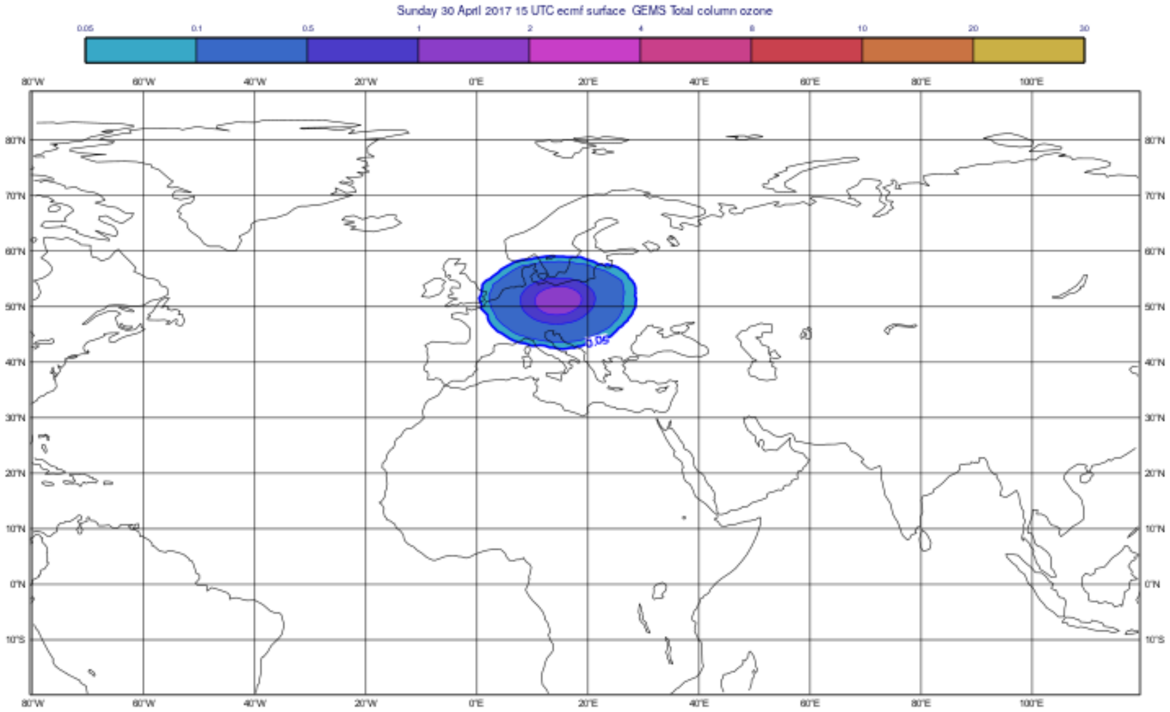


Even for those species that are observed, it is often only total column data that is available.

3. Increment from a single total column ozone observation



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

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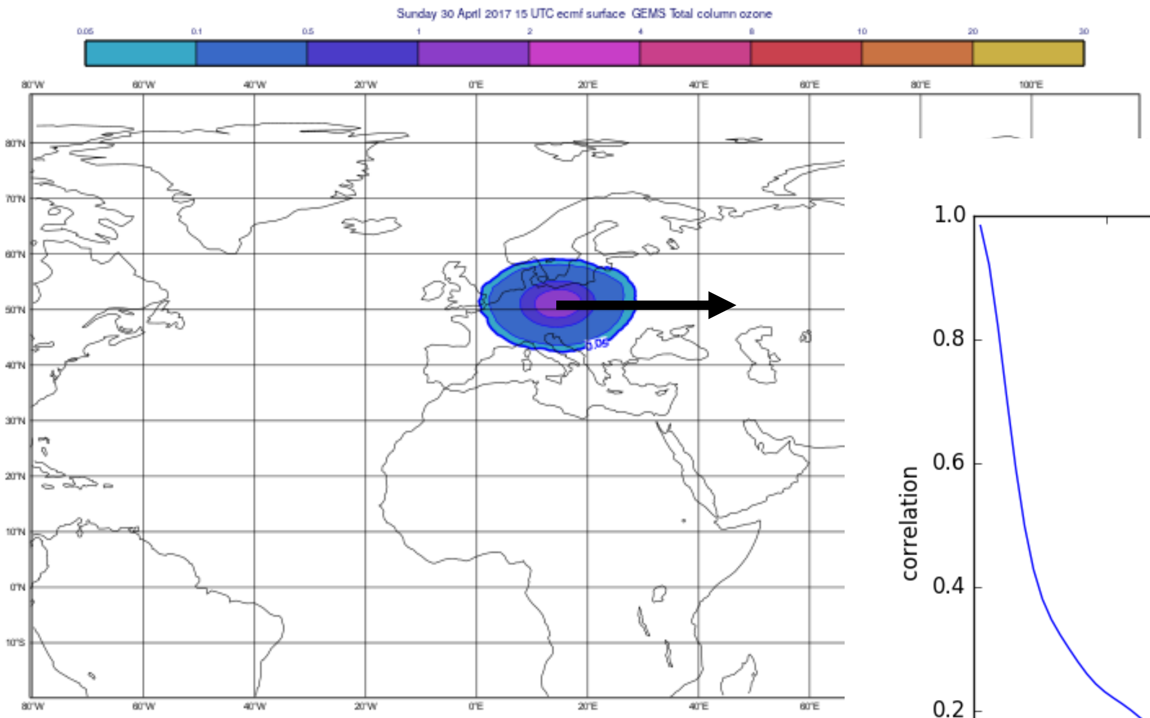

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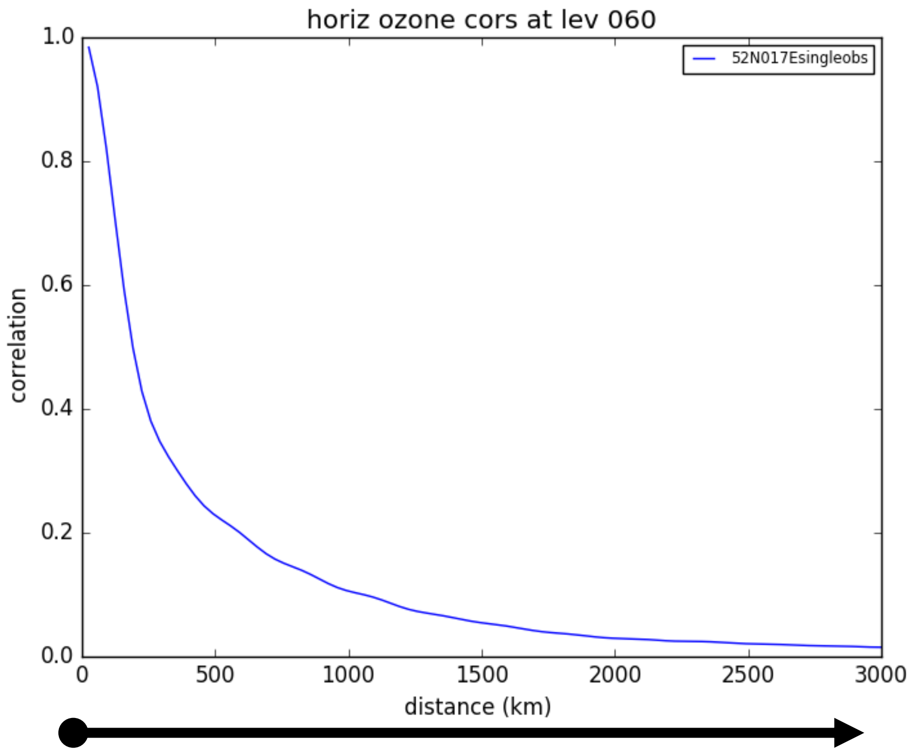

Horizontal correlation from the B-matrix that spreads the information from the single observation in the horizontal

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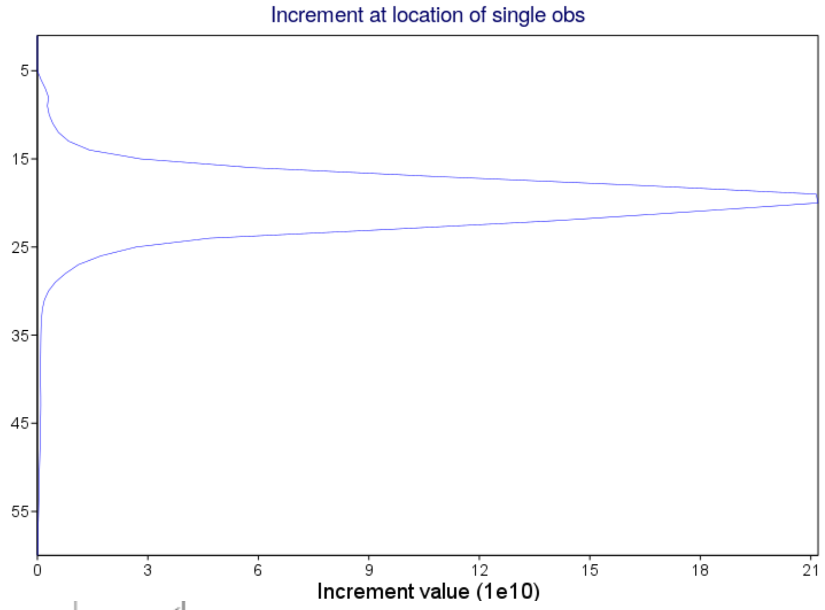
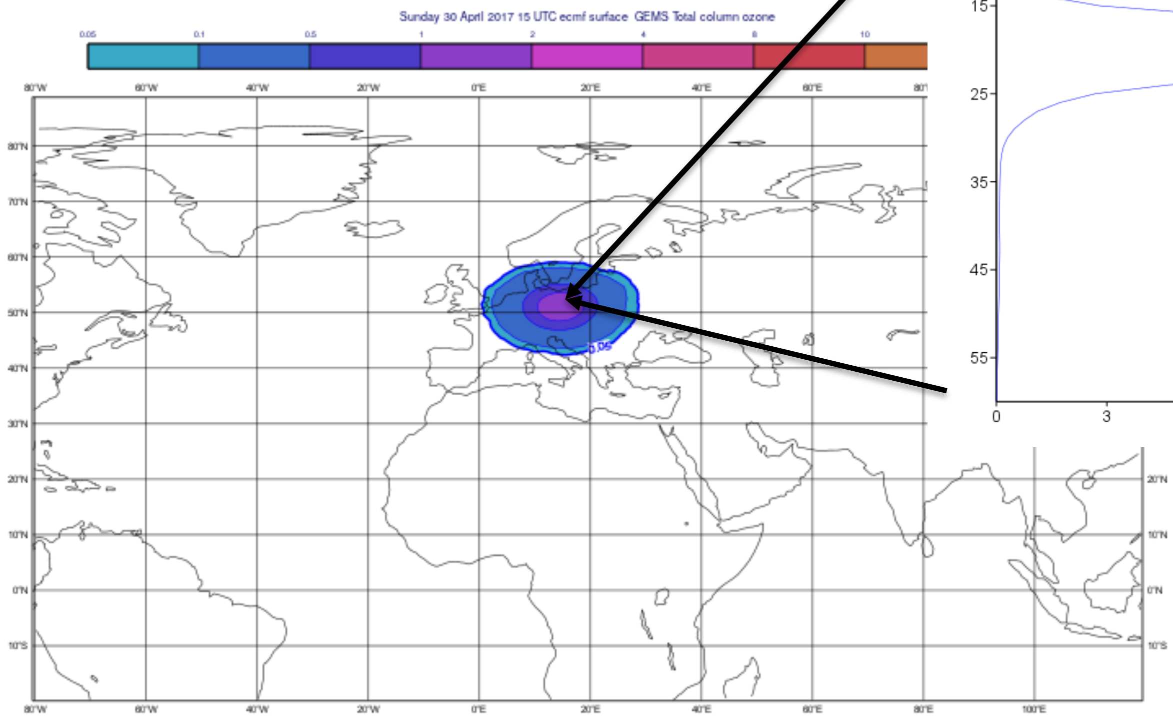
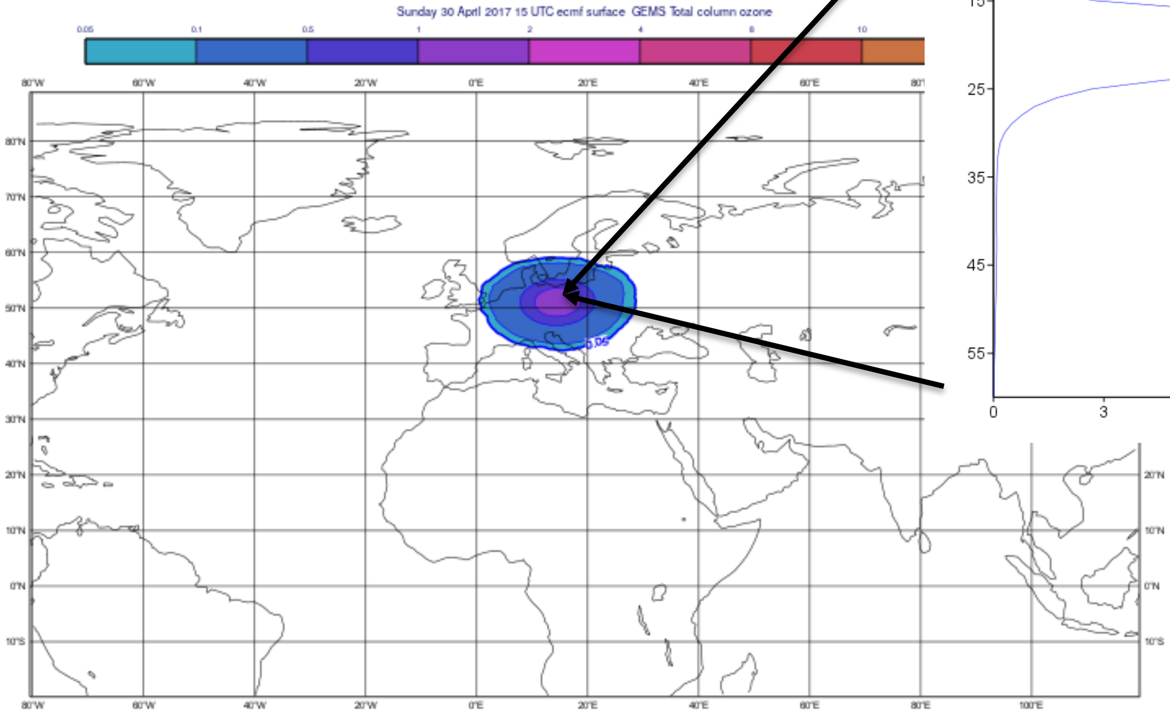


Vertical profile of the increment at the observation location

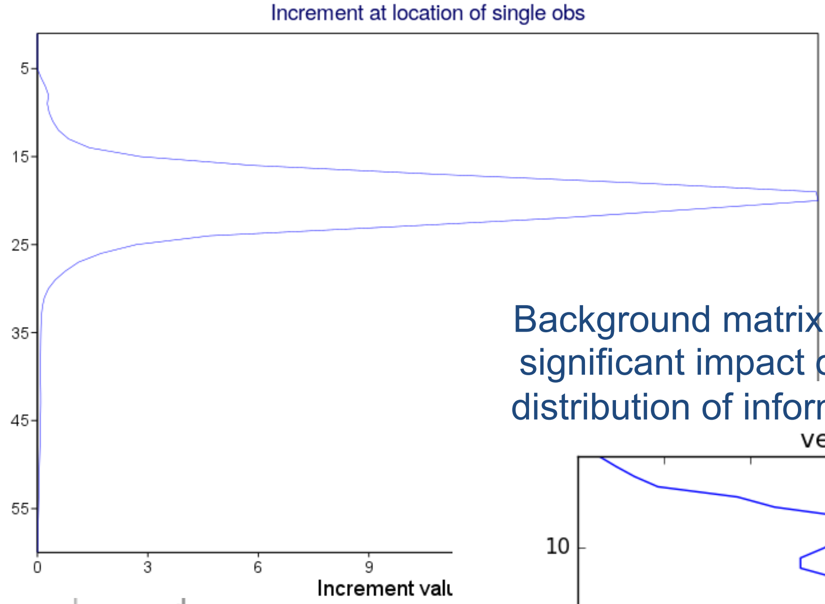


Increment created by a single ozone observation of 375 DU, 10 DU higher than background

3. Increment from a single total column ozone observation

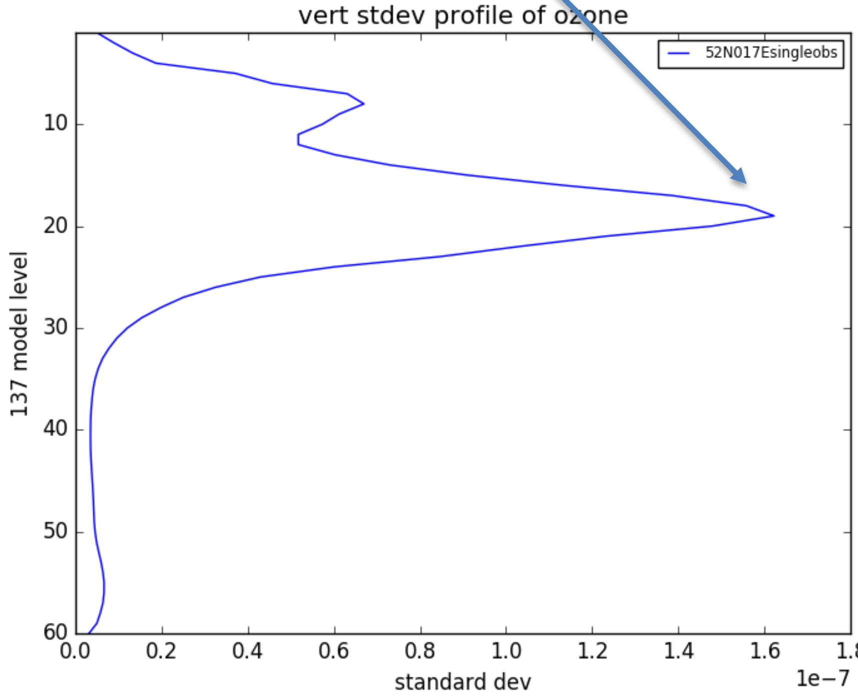


Increment created by a single ozone observation of 375 DU, 10 DU higher than background



Vertical profile of the increment at the observation location

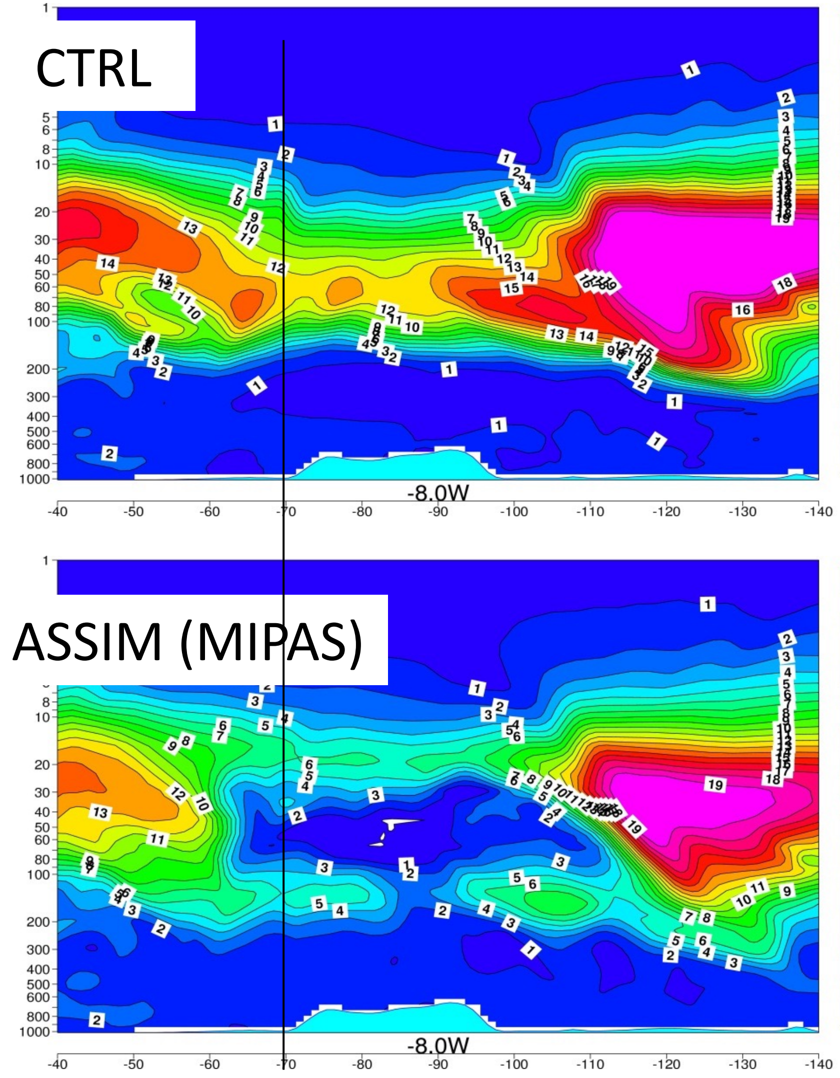
Background matrix has a significant impact on the distribution of information



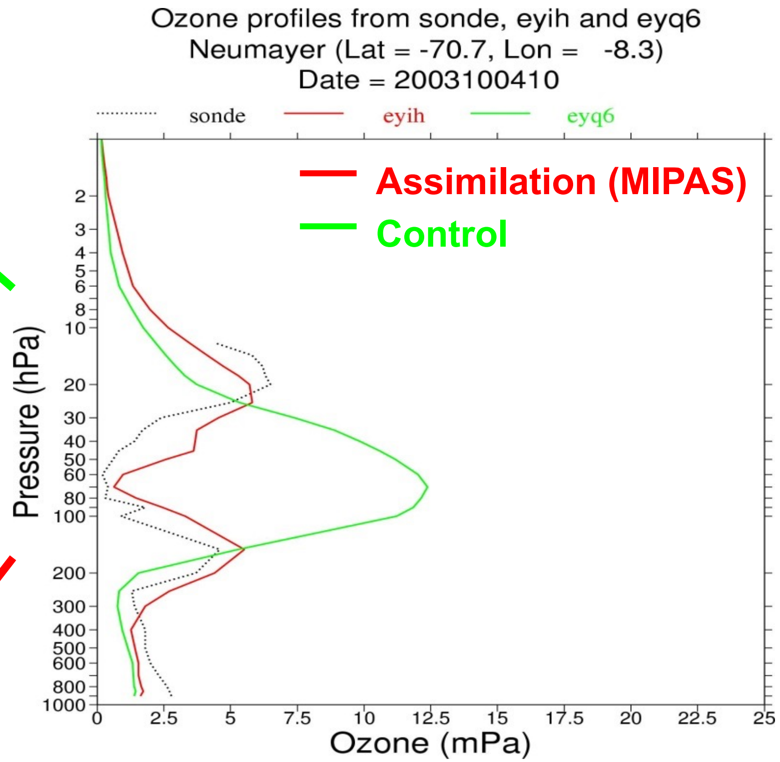
Standard deviation from the background matrix at the observation location

Formulation of the B-matrix is very important for AC

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

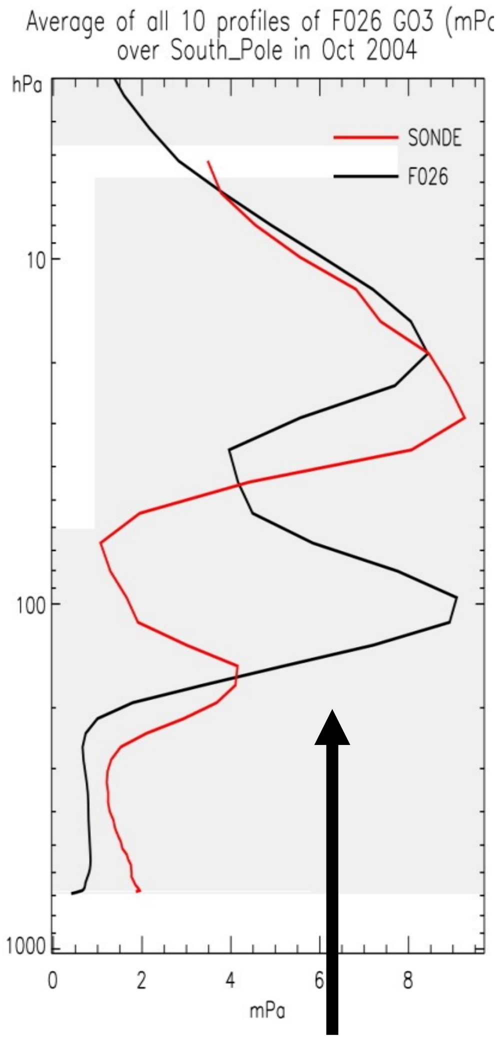


Ozone hole in CAMS reanalysis: Cross section along 8E over South Pole, 4 Oct 2003



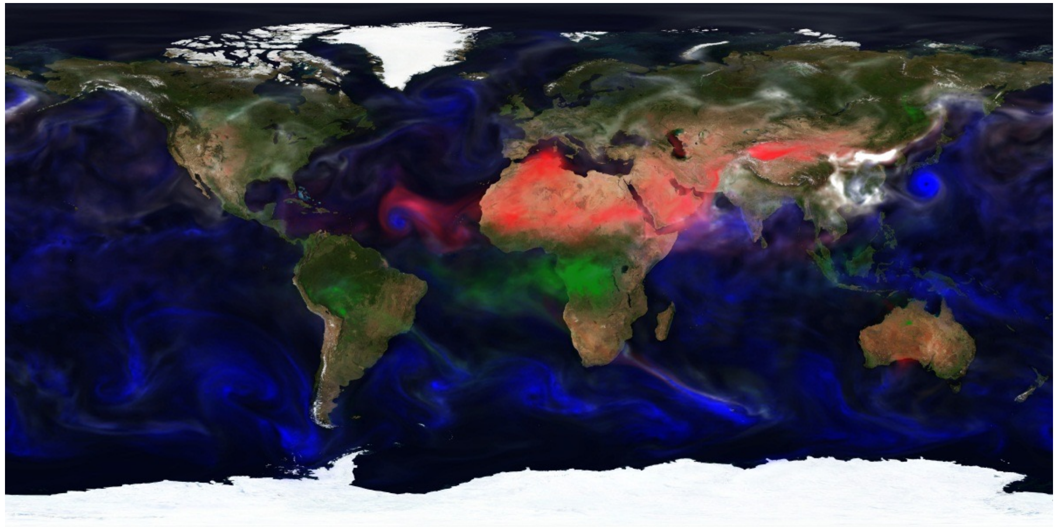
Assimilation **with profile data**

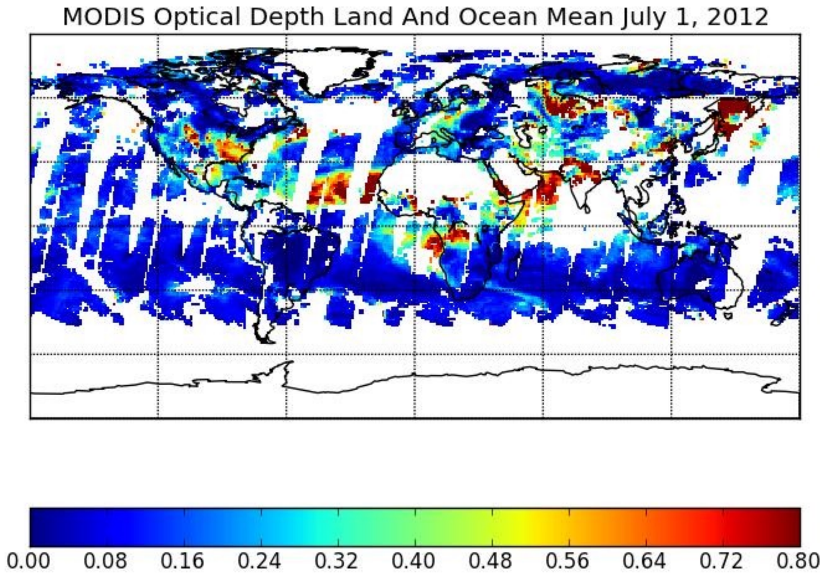
Oct 2004

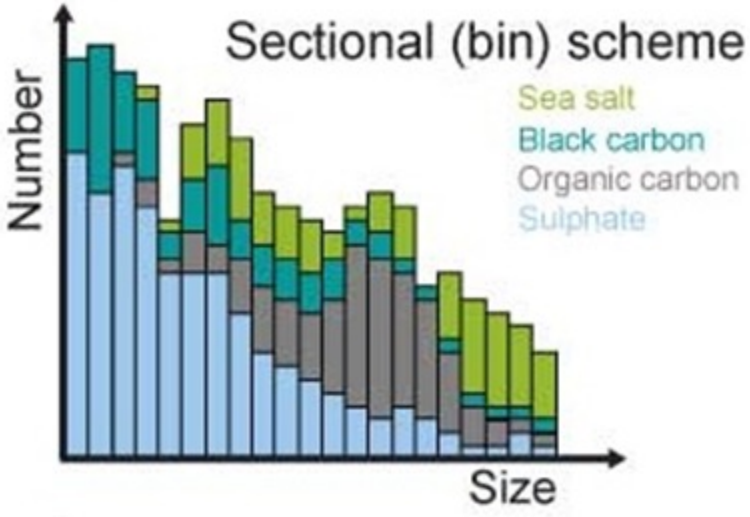


Assimilation **with total column data**

3. Aerosol – prime example of ill-observed system







Aerosol analysis

- CAMS aerosol model has 16 aerosol bins:
  - 3 size bins each for sea-salt and desert dust
  - 2 bins (hydrophilic and hydrophobic) each for organic matter and black carbon
  - 1 bin for sulphate
  - 2 bins (fine and coarse) for nitrate
  - 1 bin for ammonium
  - 2 bins (anthropogenic and biogenic) for secondary organic aerosols

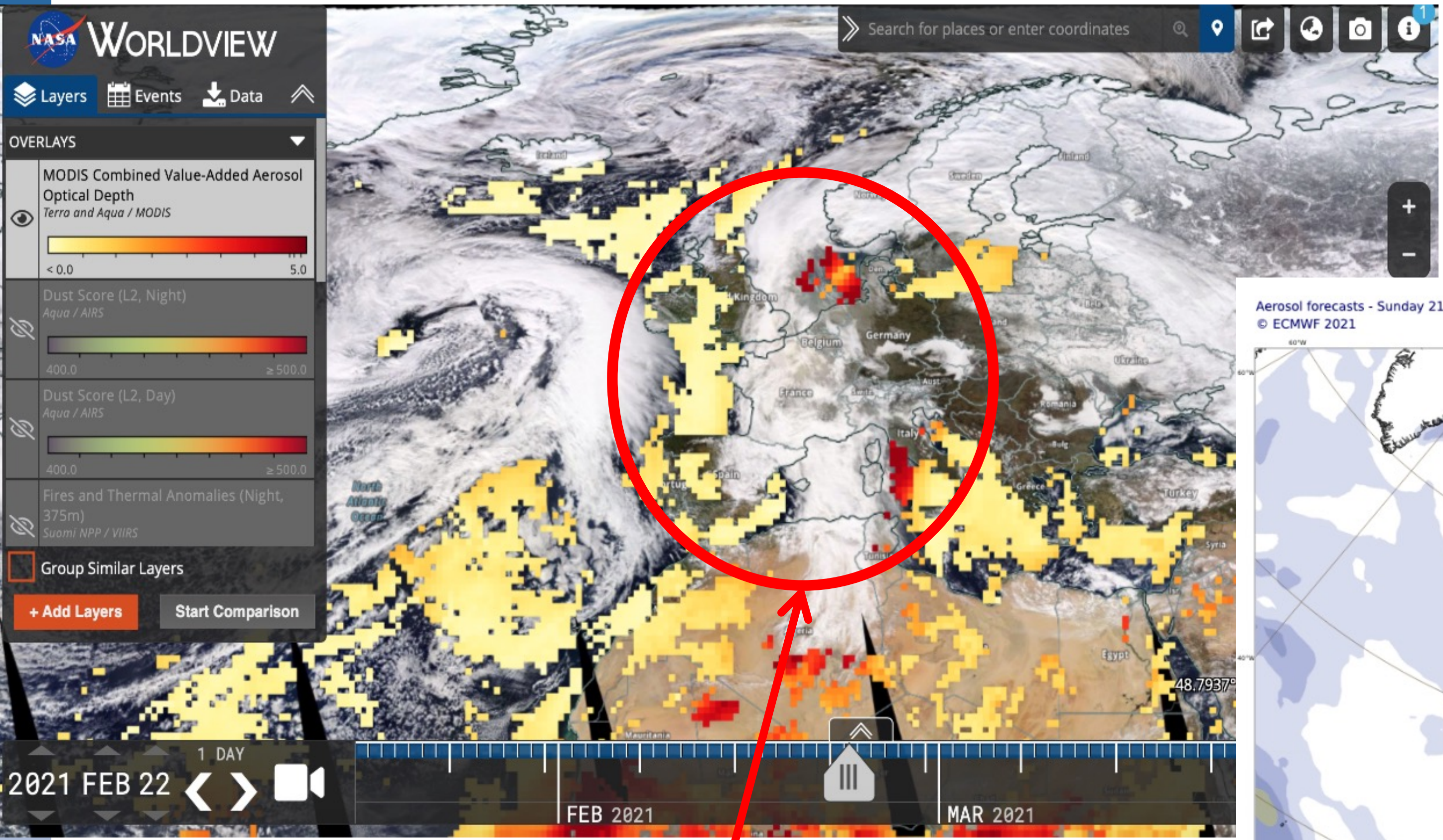
- Assimilated observations are Aerosol Optical Depth (AOD) at 550 nm from various satellite sensors. AOD is a measure of the total aerosol amount in a column.

- Control variable is formulated in terms of the total aerosol mixing ratio.

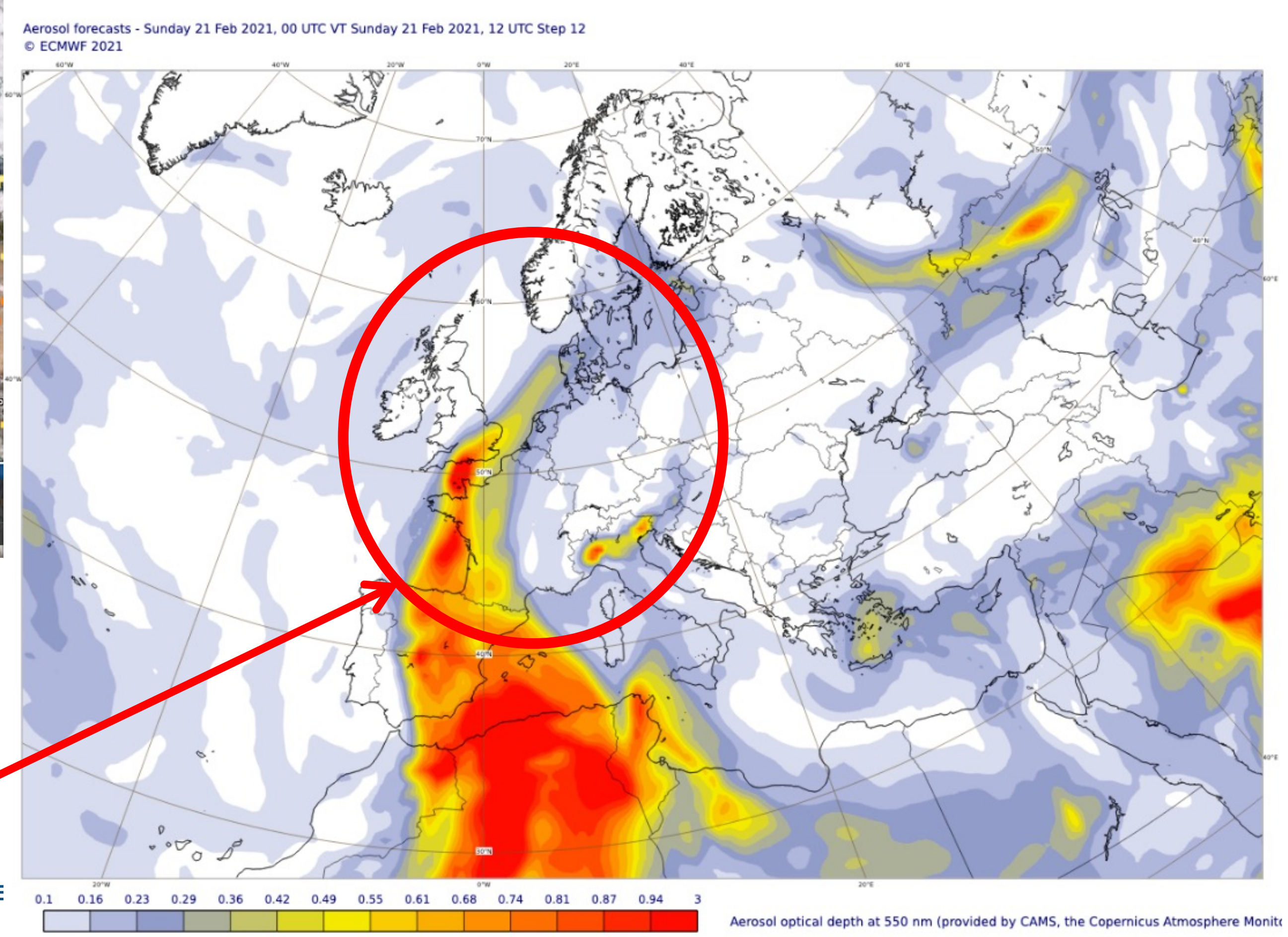
- Analysis increments are repartitioned into the species according to their fractional contribution to the total aerosol mixing ratio.

- The repartitioning of the total aerosol mixing ratio increment into the different bins is difficult

Dust storm February 2021



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



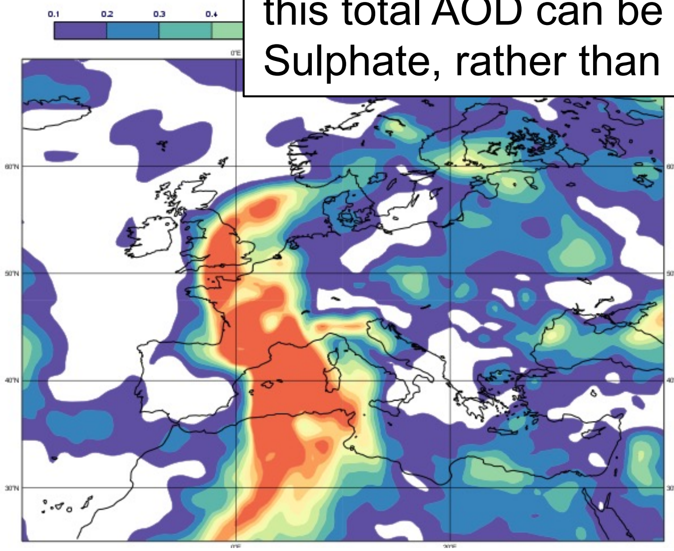
NASA Worldview – MODIS Aqua and Terra AOD 550nm observations for 20210222

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

ECMWF EUROPEAN CENTRE FOR MEDIUM-RANGE WEATHER FORE

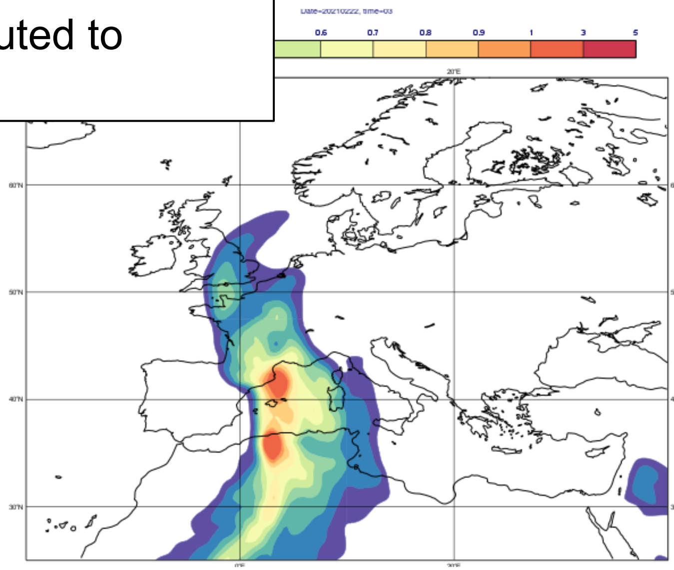
Dust test case February 2021

Closer examination shows that some of this total AOD can be attributed to Sulphate, rather than Dust

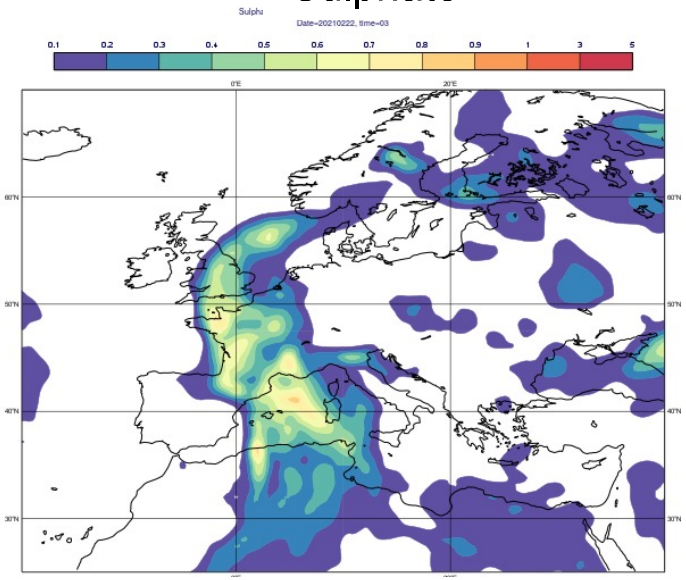


Total AOD at 550nm: 20210222 03hr

Dust

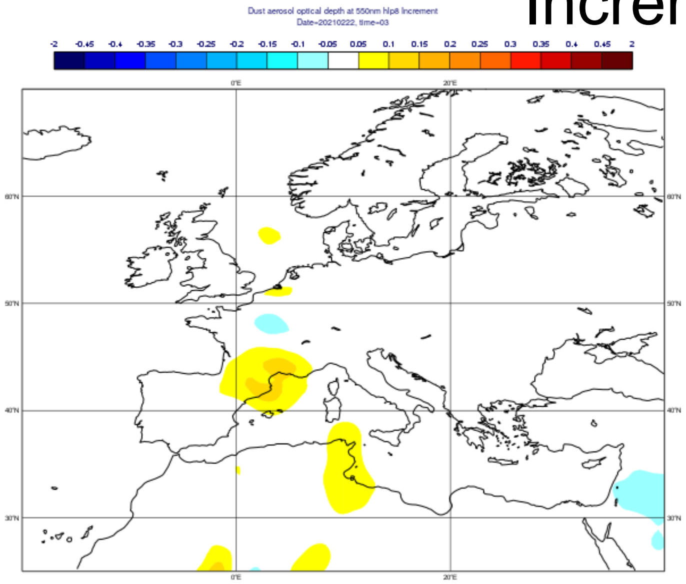


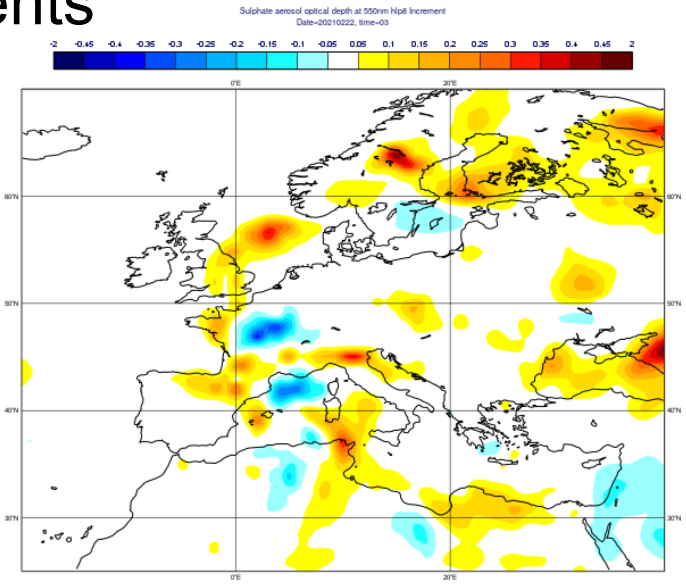
Sulphate



AOD at 550nm

Increments





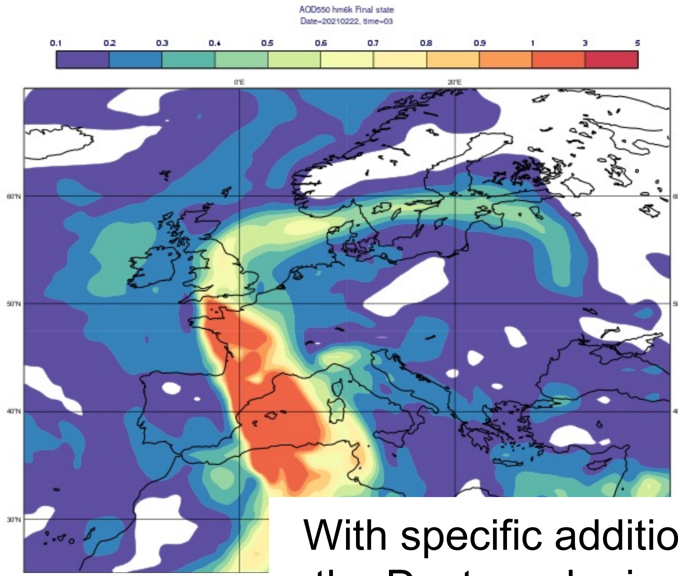
AOD incr at 550nm

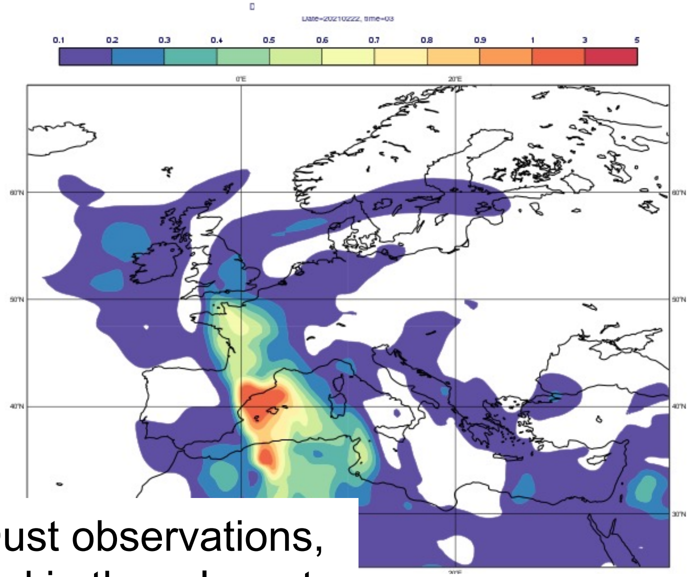
- AOD increments are attributed to the different species according to their proportion in the nonlinear forecast.
- If there is no dust in the forecast in a specific location then the increment will be given to whatever species are there – in this case Sulphate

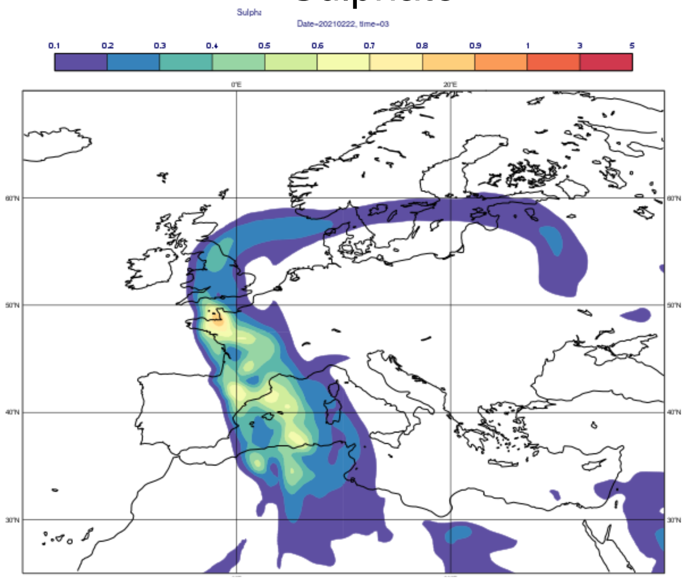
Dust test case February 2021

Dust

Sulphate

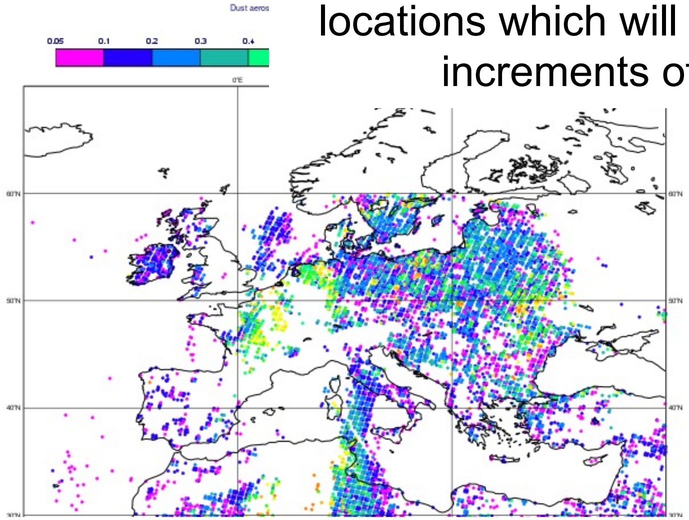




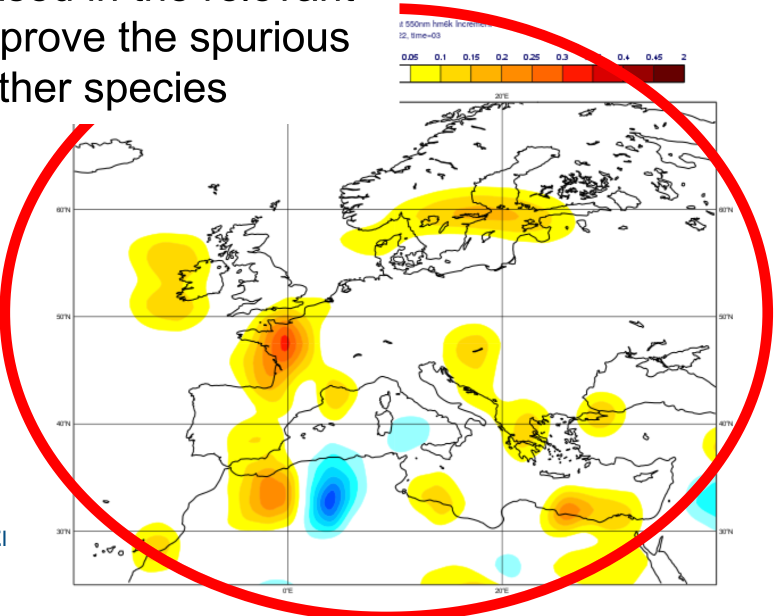


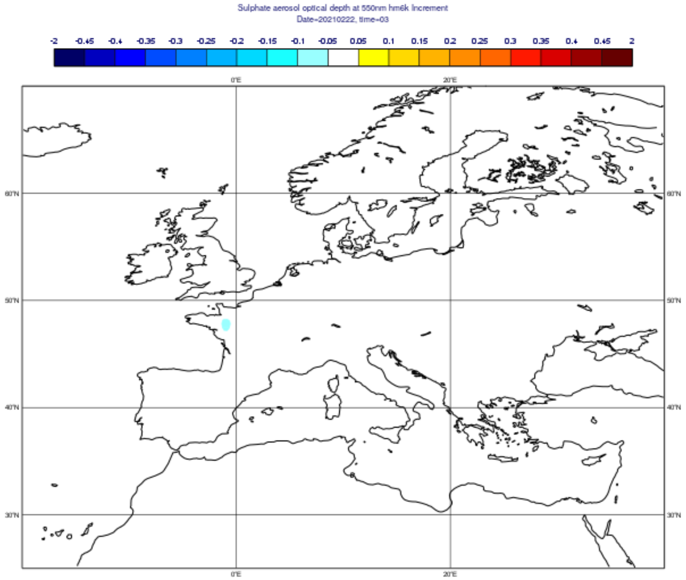
AOD at 550nm

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

Potential Benefit for NWP

Potential benefit for NWP

- Interactive aerosols: Feedback on dynamics via radiation scheme

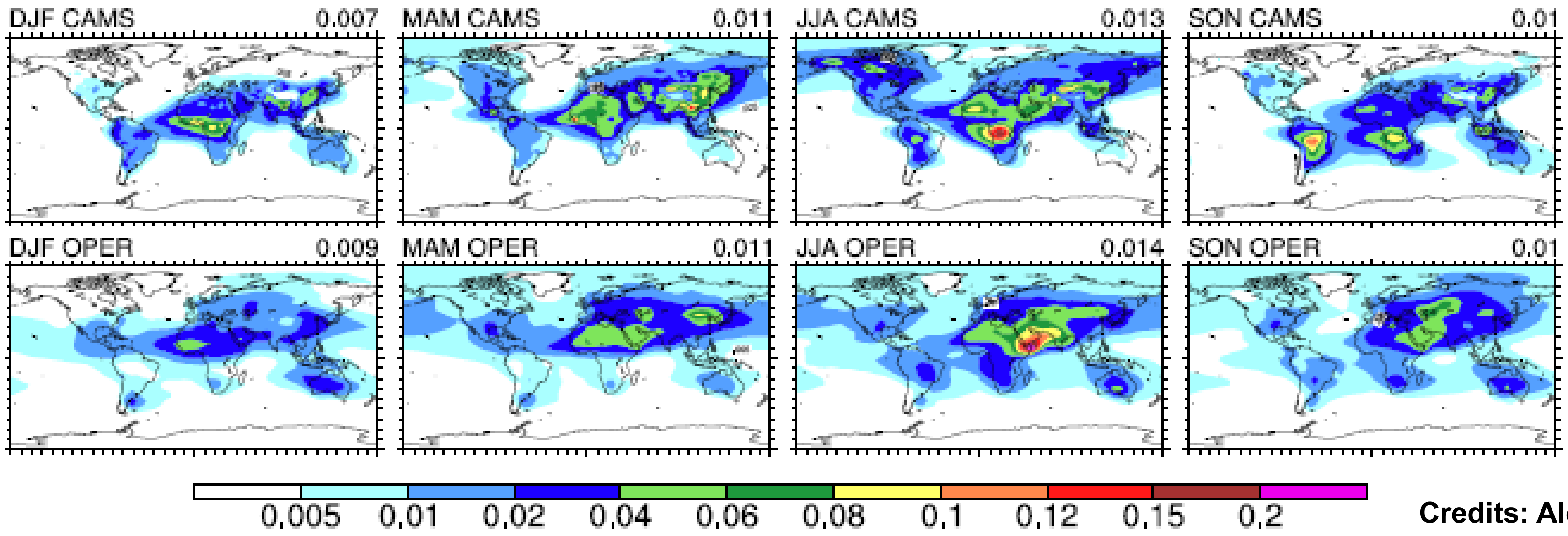
- Use of O_3 (& other fields) in the radiation scheme.

- 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.

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

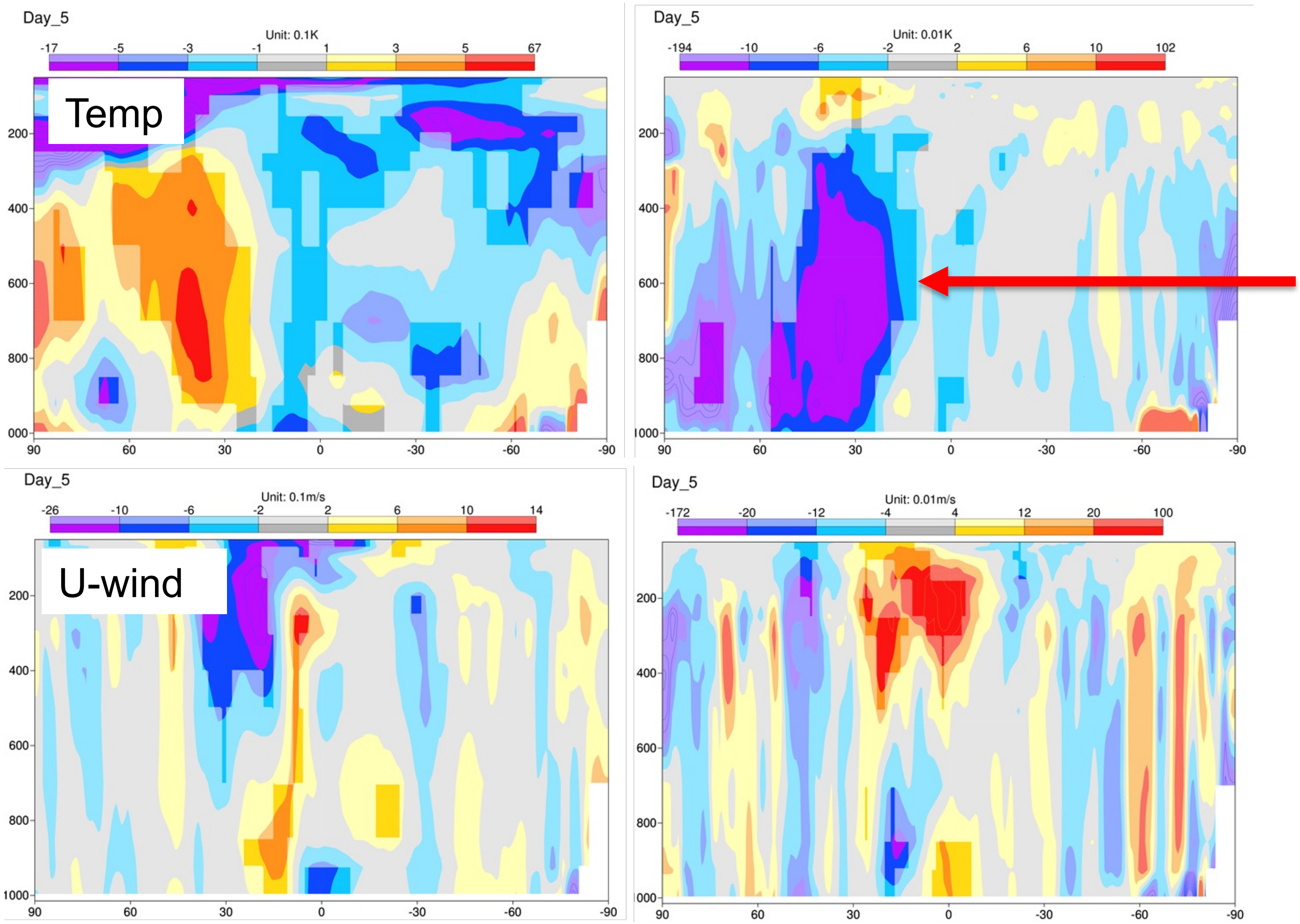
Climatological AOD 550nm distribution CAMS vs Tegen et al 1997



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



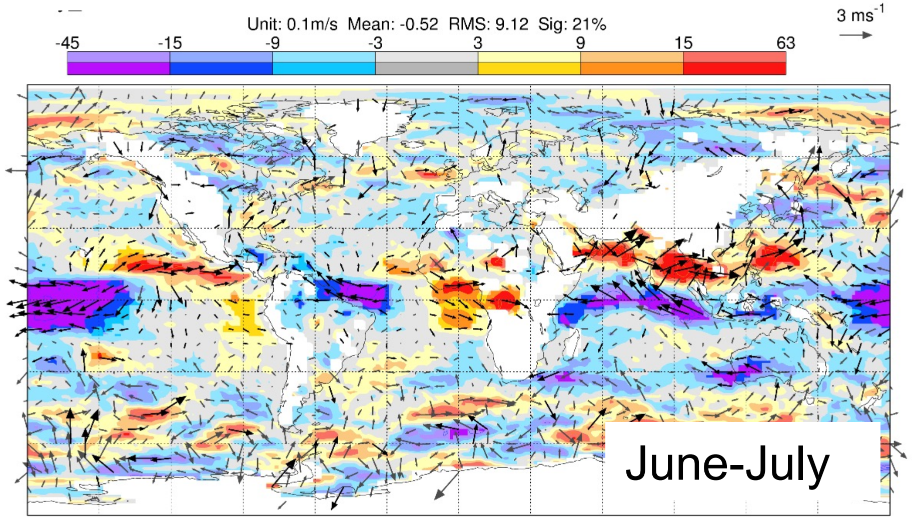
June-July
Model FC error d+5

June-July
Change in FC error d+5

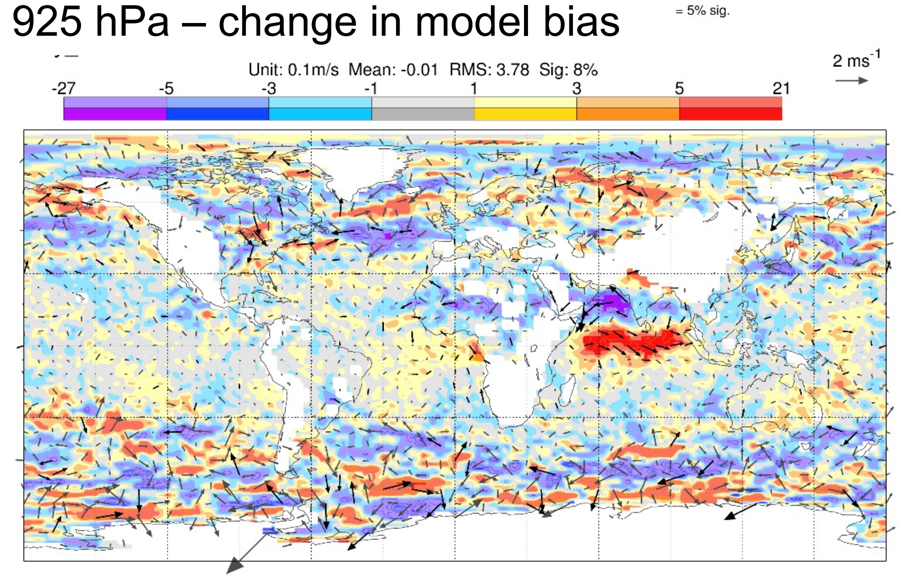
- Change in mass distribution and optical properties -> reduction in SW absorption -> reduction in temperature (positive)
- This is of the order of 0.1K for a bias of the order of 0.3K – it explains at least ~30% of the temperature error.
- Similar for winds at upper levels

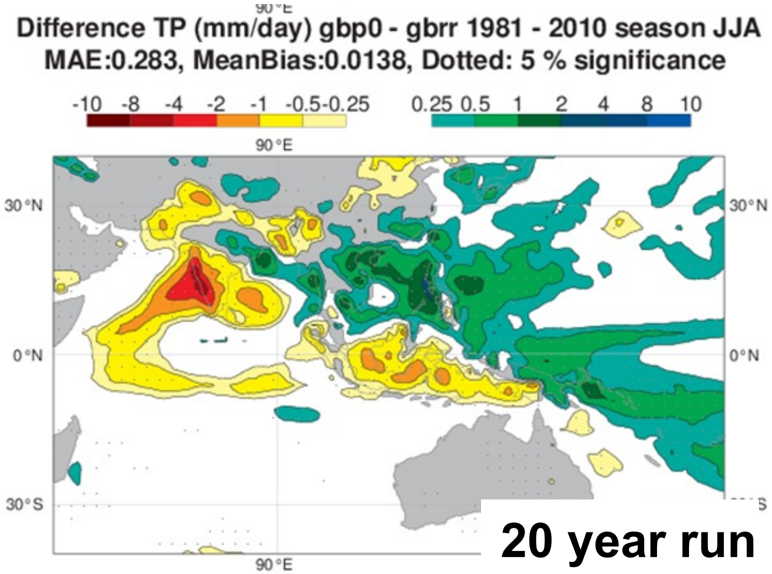
Improvements to NWP forecast errors

U 925 hPa – model bias at D+5

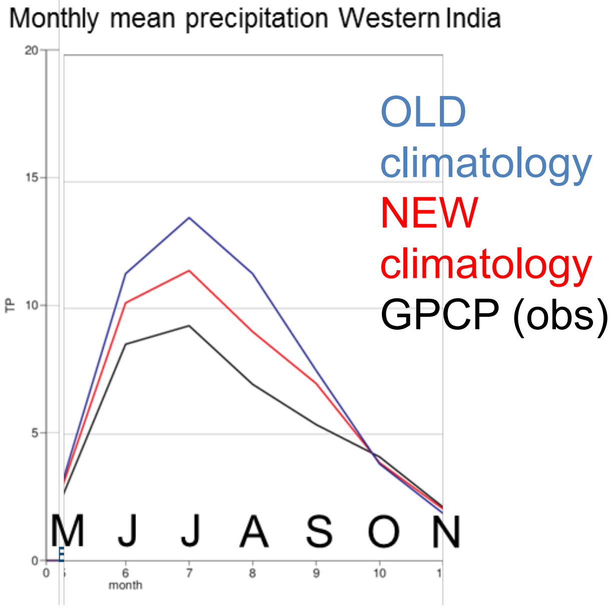


U 925 hPa – change in model bias





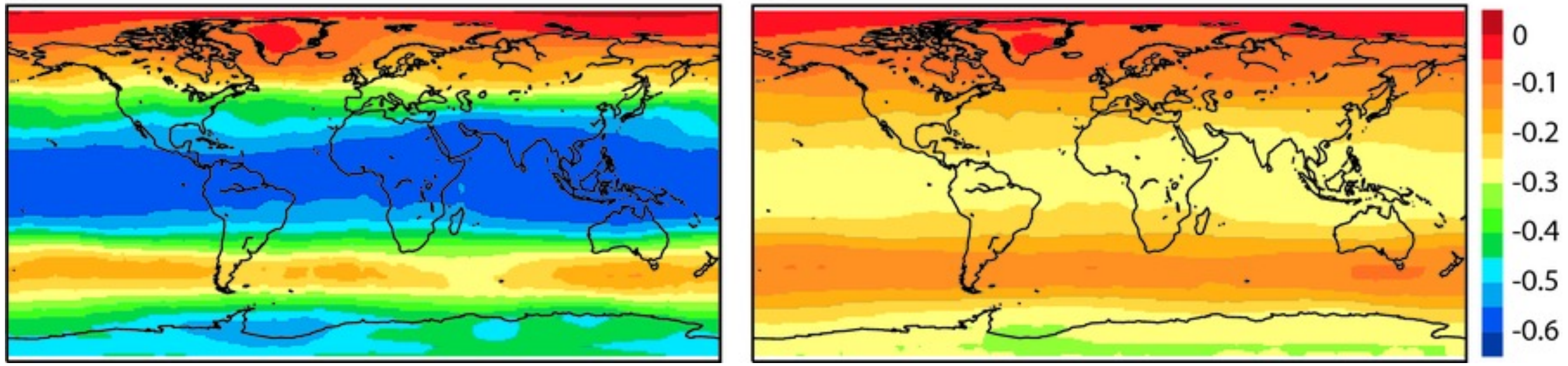
Too strong monsoon circulation in Indian Ocean in the model leads to too high precipitation over west India.



Revised aerosols affect the circulation and reduce the bias both in the wind circulation and in the precipitation amounts in Summer

Benefit of AC for NWP: Variable CO2 in radiance assimilation

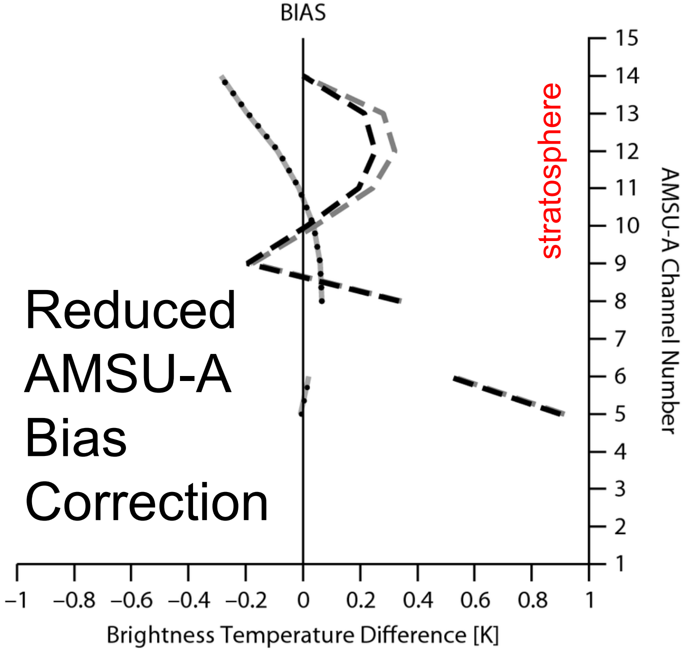
Reduced AIRS and IASI Bias Correction



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

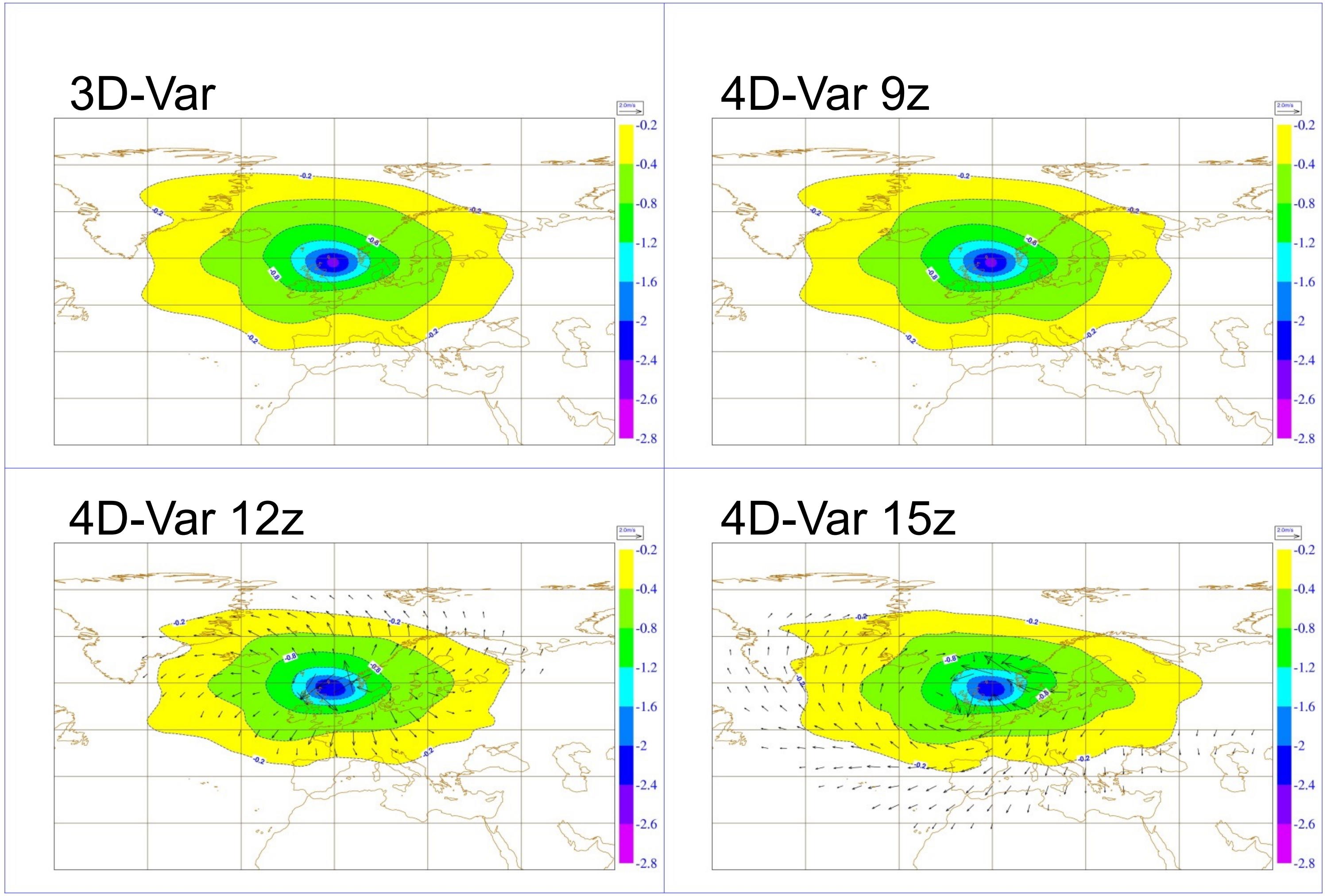
- Using modelled CO_2 in AIRS/IASI radiance assimilation leads to significant reduction in needed bias correction.
- Small positive effect on T analysis and neutral scores/ small positive impact at 200 hPa T in Tropics
- Stratospheric T in variable CO2 exp more consistent with AMSU-A
- It would be beneficial 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.
- Similar to cloud track winds but data coverage worse.
- Potential to extract wind info indirectly through TL and AD of tracer advection
- 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

Single observation experiments - Ozone and wind increments



Level 20,
≈ 30 hPa

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

Observation at T3: wind increments

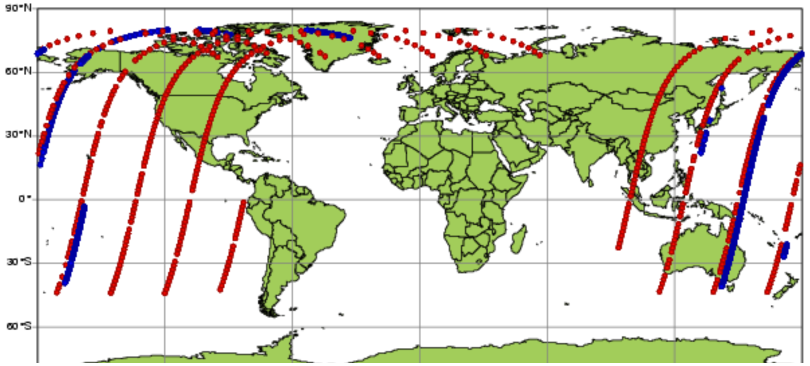
Observation at T6: wind increments

6h assimilation window

Benefit of AC for NWP: Requirements to extract wind info from tracers

- Complete data coverage (3D), frequent observations.
- Accurate observations
- High quality background field
- No bias between observations and background
- Depends on accuracy of TL model compared to full model (better for passive tracers/ long chemical lifetime) => E.g. extracting wind information from O_3 is more difficult in the tropics and summer hemisphere where photochemical lifetime is shorter
- Studies have looked at this in idealized experiments (e.g. Daley 1995; Riishojgaard 1996; Peuch et al. 2000; Allen et al. 2013, 2014) focussing on long lived tracers O_3, H_2O, N_2O and found positive impact for perfect observations.
- Few studies used real data (e.g. MLS O3, Semane et al. 2009) and positive results are less clear

Benefit of AC for NWP: Example from ERA-Interim



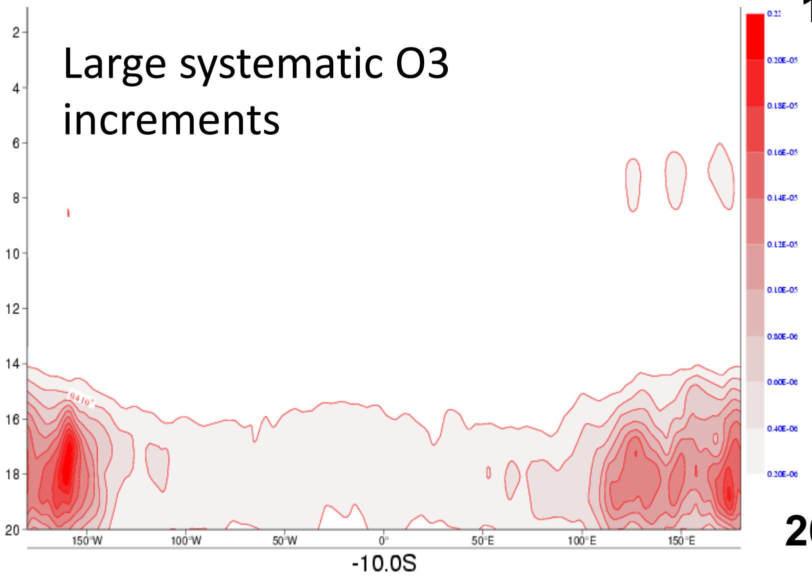
GOME 15-layer profiles (~15,000 per day)
SBUV 6-layer profiles (~1,000 per day)

The stratosphere is not well constrained by observations:

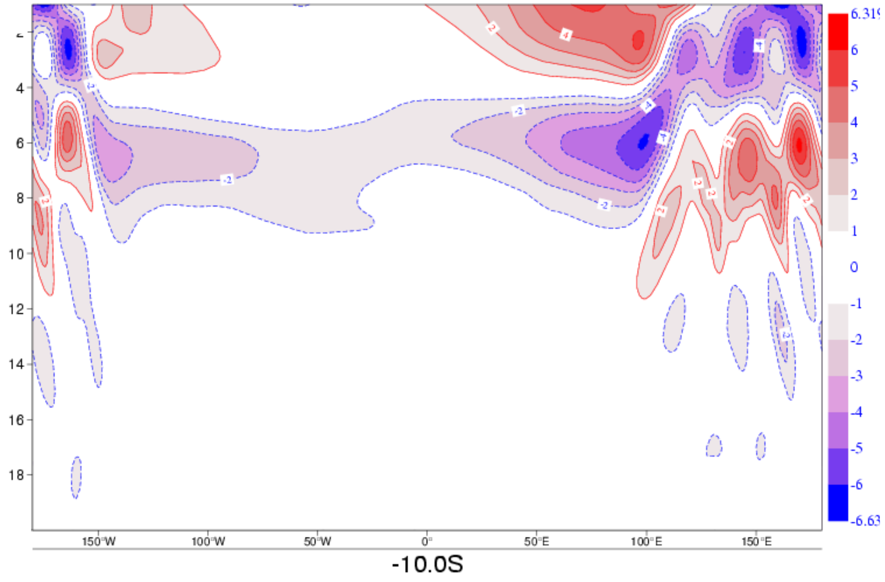
- Ozone profile data generate large temperature increments
- 4D-Var adjusts the flow where it is least constrained, to improve the fit to observations

=> IFS O3 analysis is completely uncoupled now

Ozone increments at 10S



Associated Temp increments



D. Dee

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 off

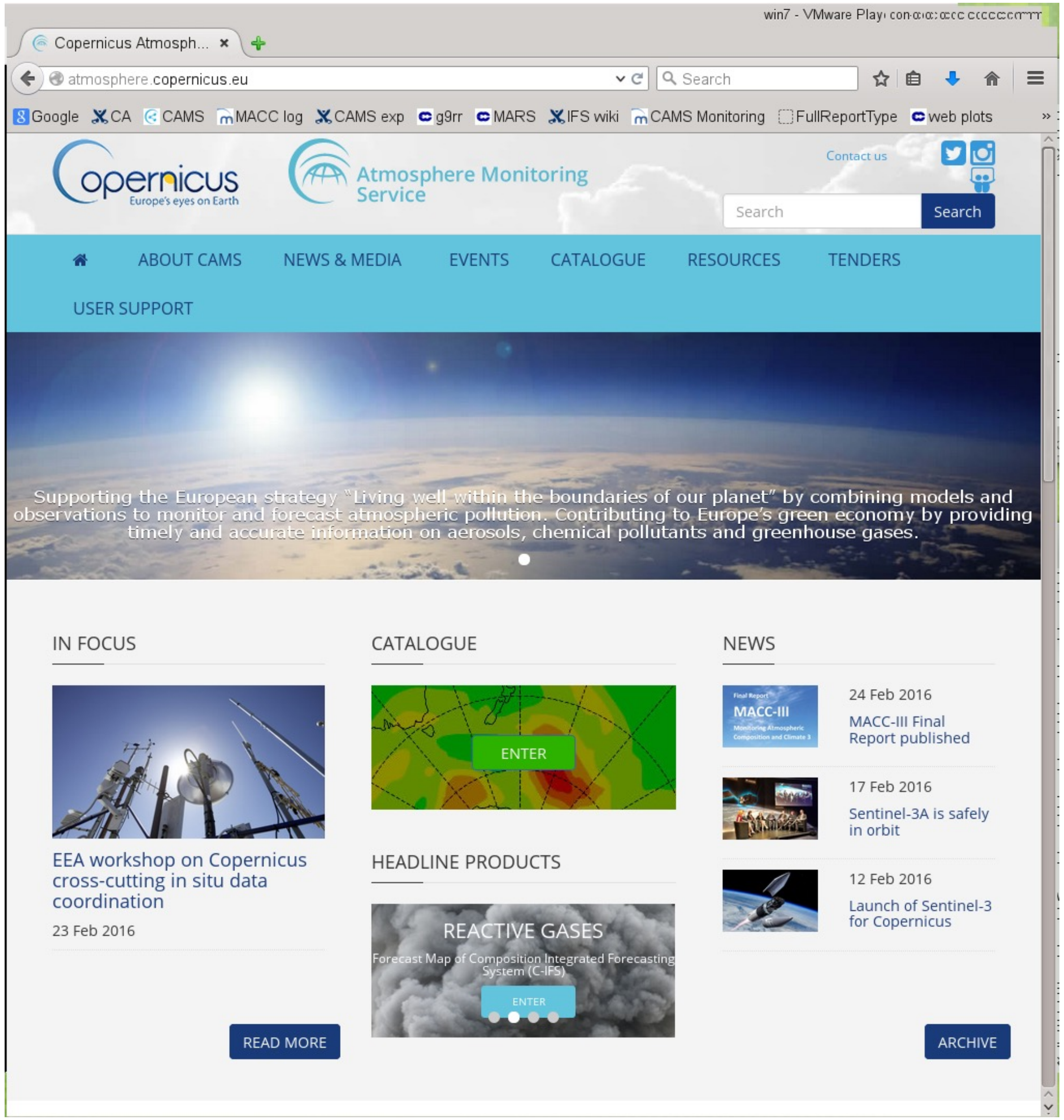
Summary

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 life time of some species
- Atmospheric composition has the potential to improve various aspects of NWP
- 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



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