Data assimilation of atmospheric composition

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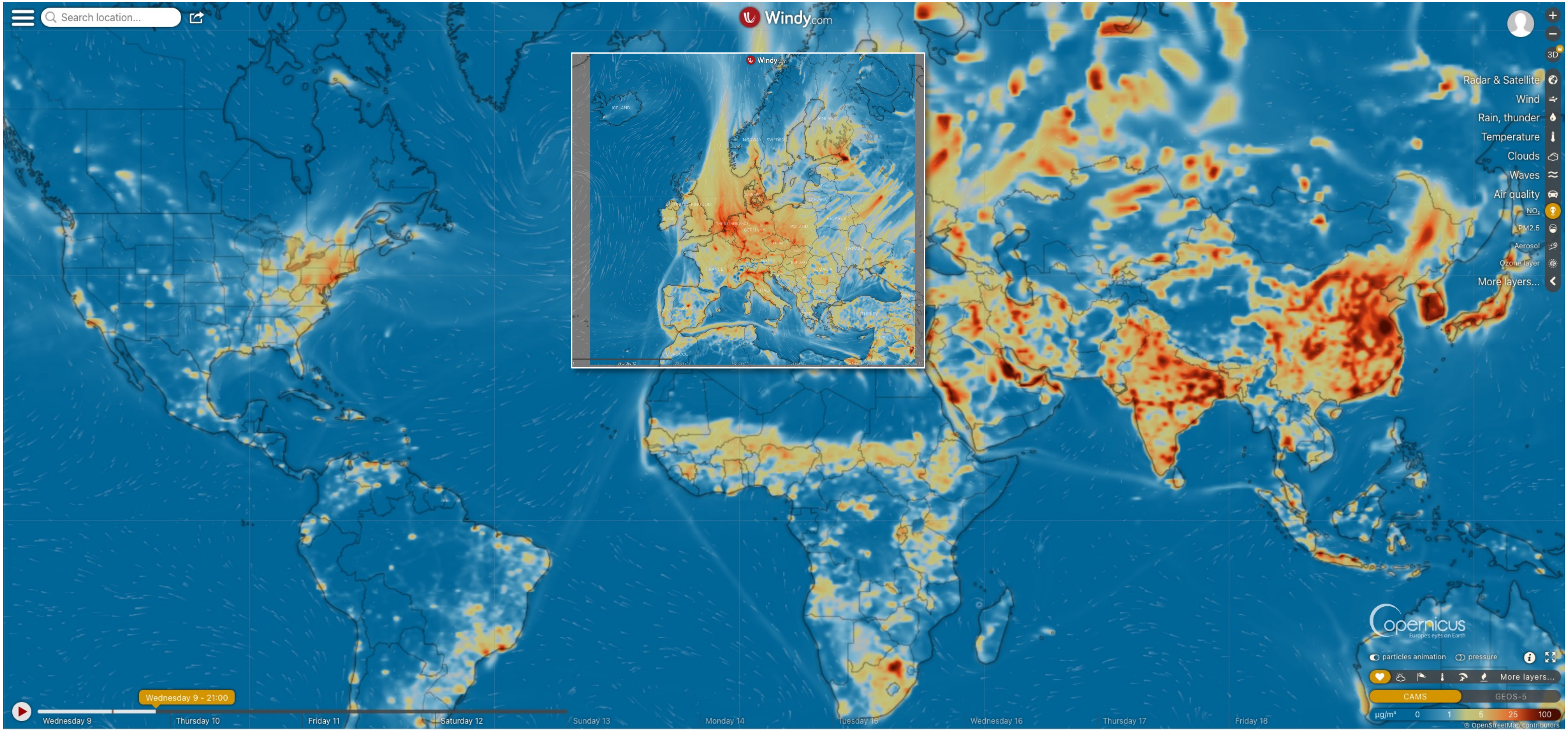
Why atmospheric composition at an operational weather prediction centre?

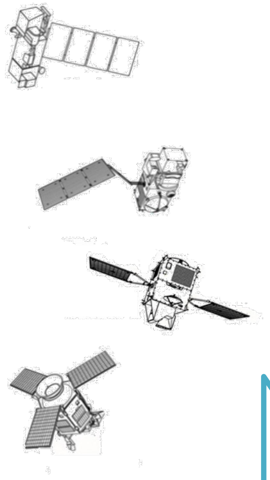
- Poor air quality is a major public health issue in many countries.
- Local authorities need accurate and timely information to implement effective air pollution mitigation measures.
- Accurate air quality forecasts require accurate transport models.
- Can leverage sophisticated data acquisition infrastructures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

Real-time air quality forecasting services

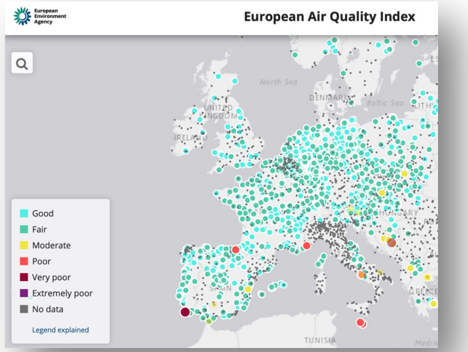


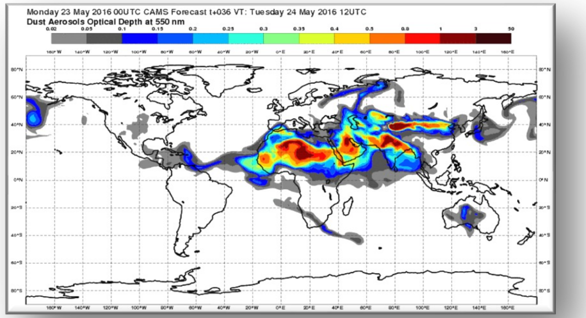
Copernicus Atmosphere Monitoring Service

Atmosphere Monitoring Service
atmosphere.copernicus.eu



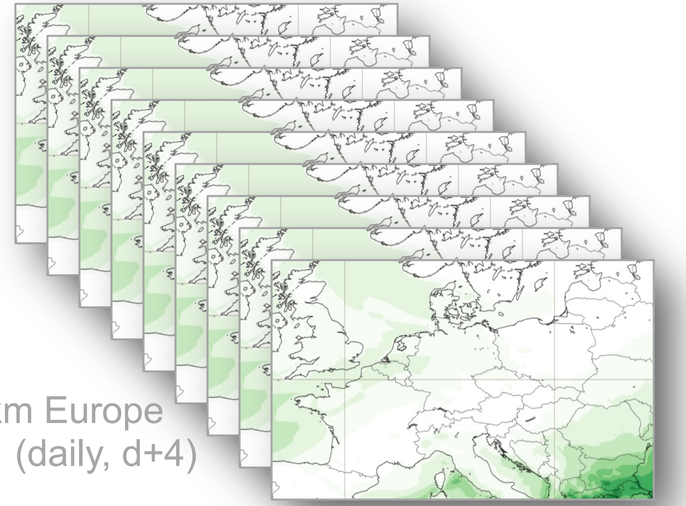
Earth Observation from satellite (>80 instruments) and in-situ (regulatory and research)





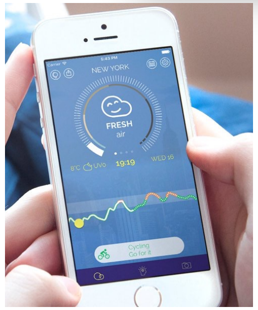
40km Globe (twice daily, d+5)

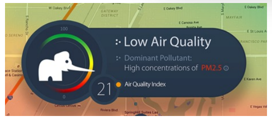
CAMS main operational **data assimilation and modelling systems**



10km Europe (daily, d+4)

CAMS users
>22,500
(>2600 routine)



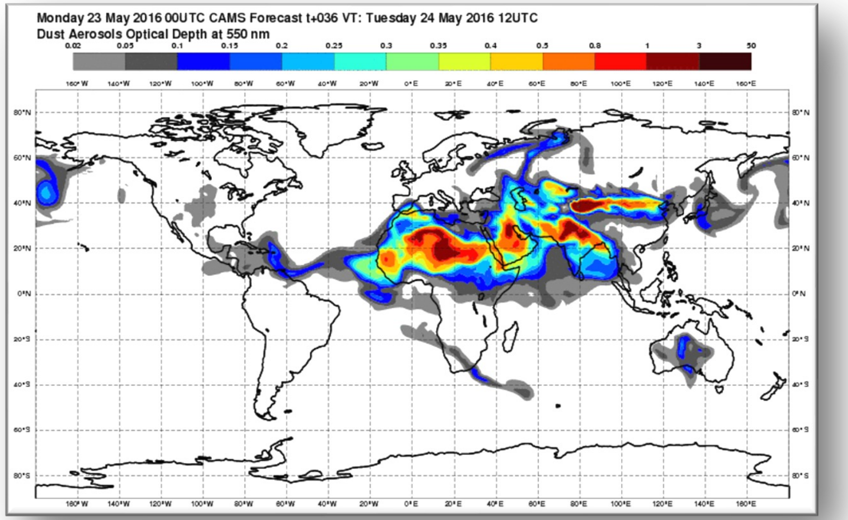


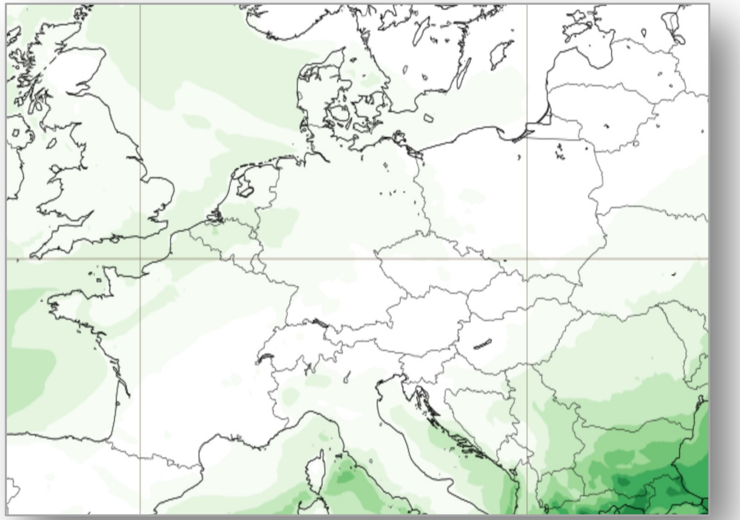
Windy.com

The Weather Channel

ECMWF EUROPEAN CENTRE FOR MEDIUM-RANGE WEATHER FORECASTS

Atmospheric composition DA - some constraints to start with





Global models

- Well-adapted to satellite data
- In-situ data often too sparse or not providing good global coverage
- Focus on long-range transport and less on surface air quality

Regional models

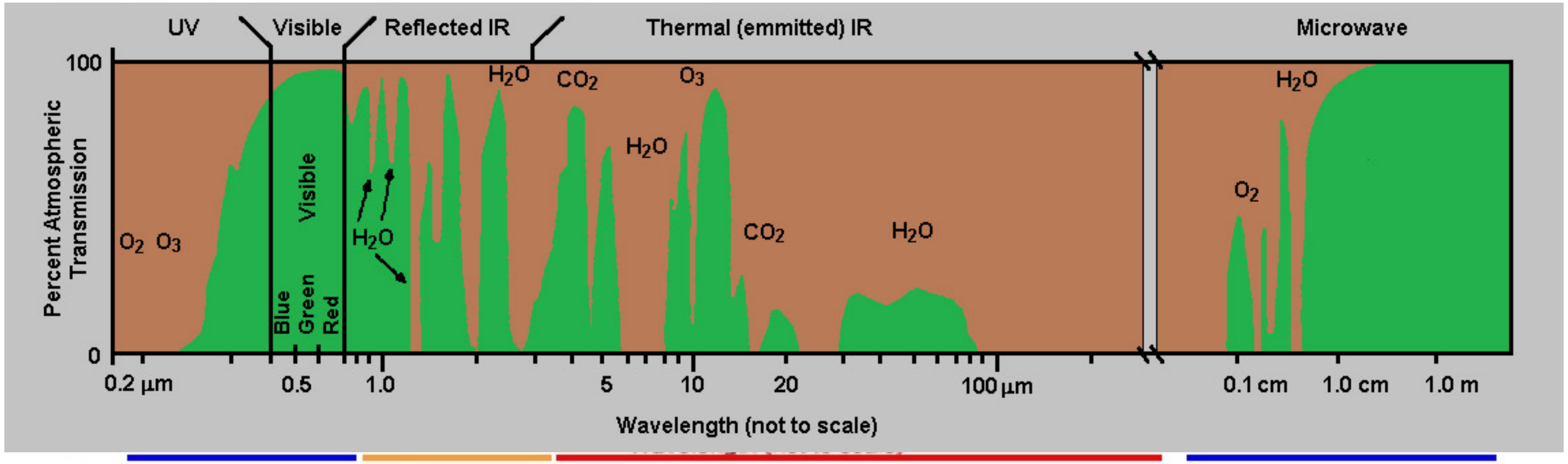
- Well-adapted to in-situ data, although timeliness can be a problem
- Satellite data more difficult to use due to limited vertical domain
- Focus on surface air quality, but will need long-range transport as boundary condition

What can we actually observe?

Focus on satellite observations for a global forecasting system

Spectral signature of trace gases

NIR, SWIR



O_3
H_2O
NO_2
SO_2
H_2CO, $C_2H_2O_2$
IO
BrO

CO_2
CH_4
CO

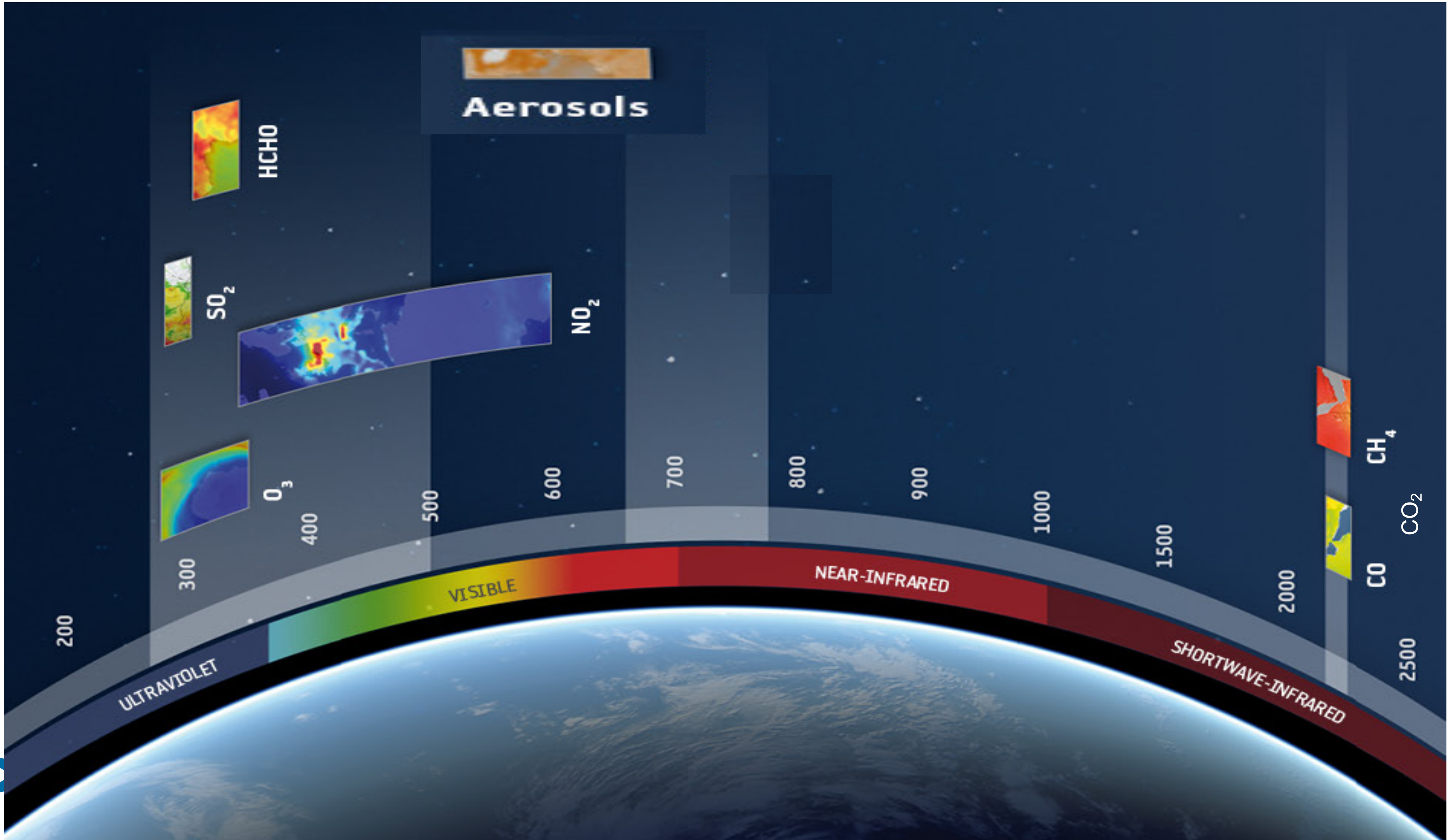
H_2O
CO_2
CH_4
N_2O
O_3
CO
HNO_3
NH_3
CFC11, CFC12, …
CH_3OH, HCOOH, C_2H_2, C_2H_6,…
+ isotopologues

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

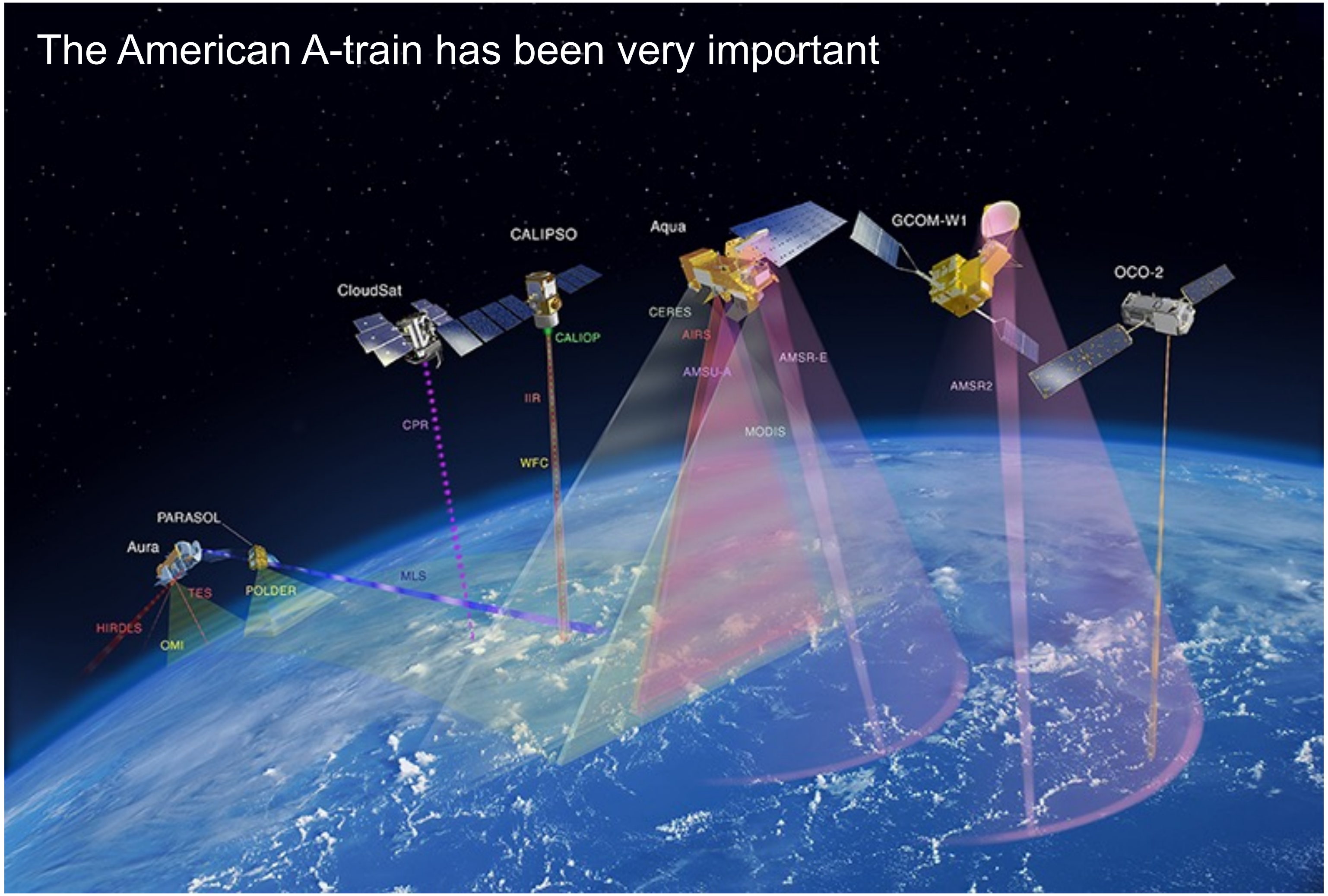
Credit: M. Van Roozendael

Spectral bands and different species observed

UV to SWIR



Satellite observations



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

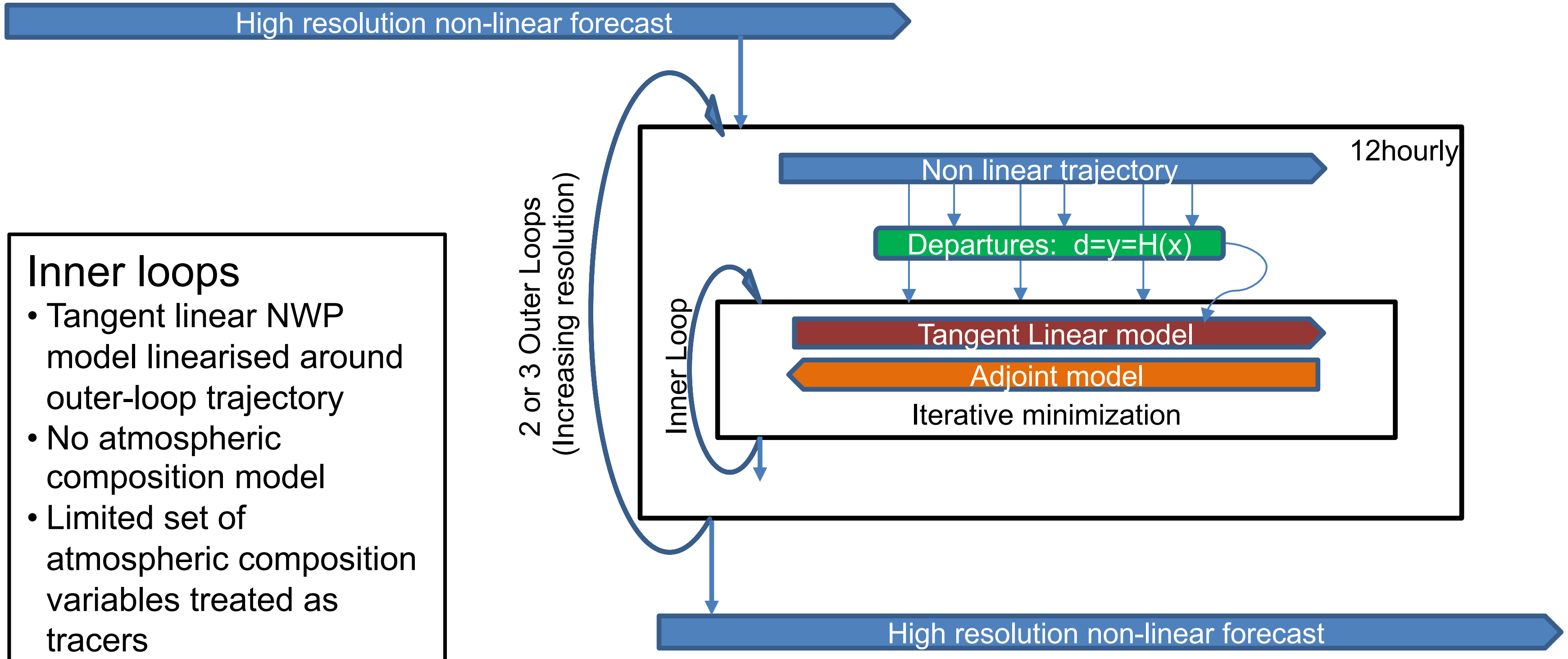
Around 20 different data streams are operationally assimilated or monitored into IFS on top of the meteorological data streams.

Data assimilation methodology for atmospheric composition

Data Assimilation Methodology

Data assimilation for atmospheric composition is in principle not different from NWP data assimilation

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



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

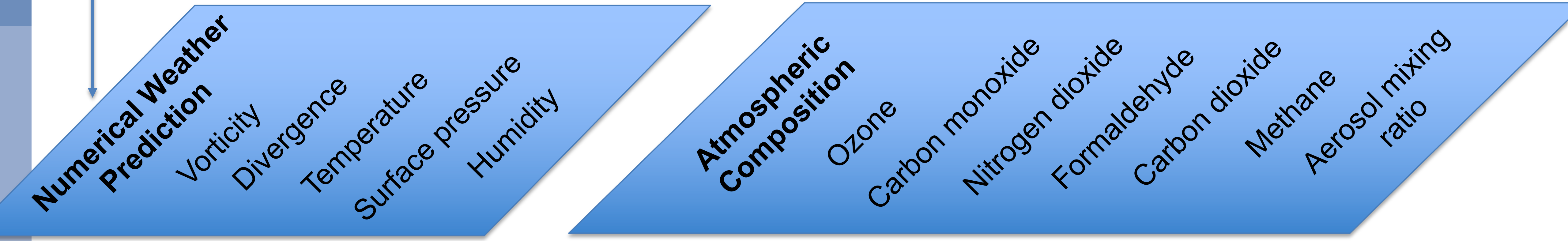
Inner loops
- Tangent linear NWP model linearised around outer-loop trajectory
- No atmospheric composition model
- Limited set of atmospheric composition variables treated as tracers

Incremental 4D-Var

Data Assimilation Methodology

Data assimilation for atmospheric composition is in principle not different from NWP data assimilation

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

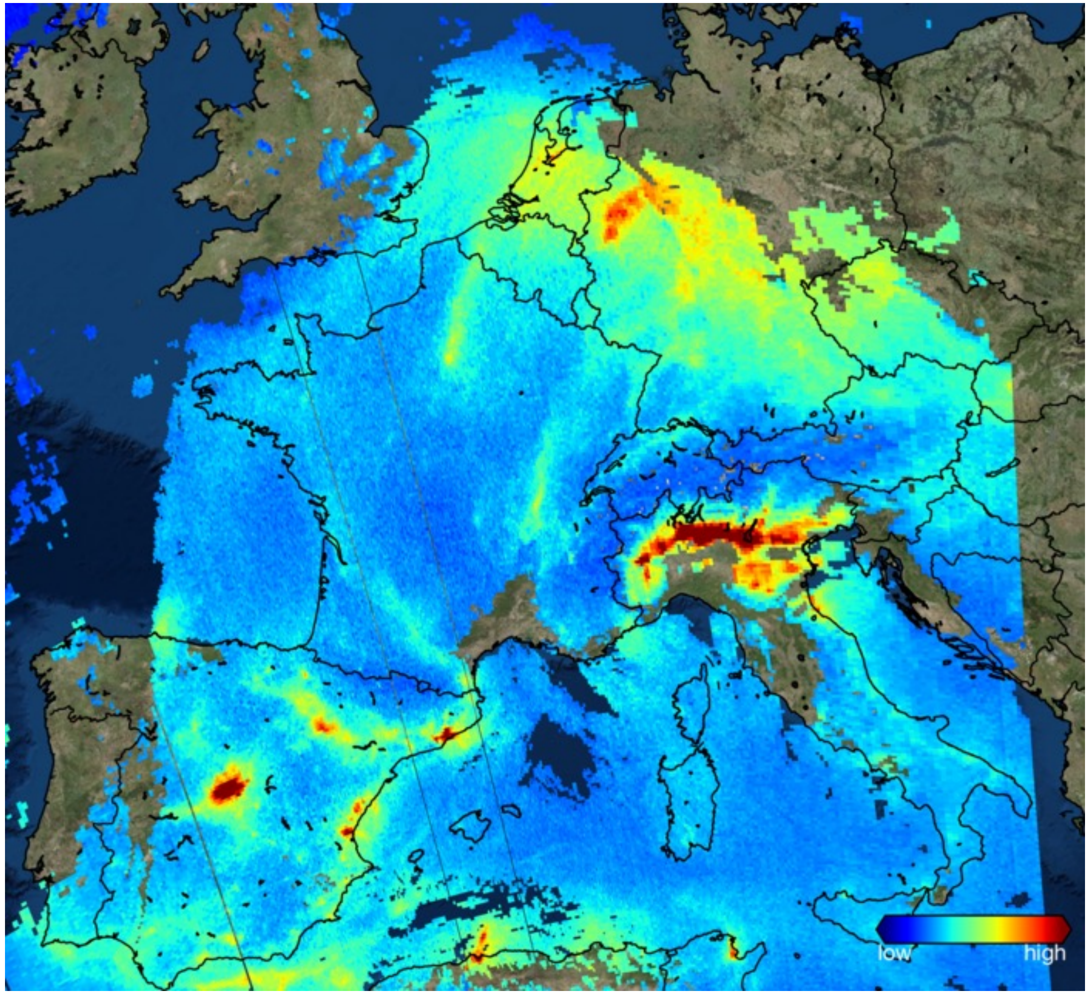


$$\mathcal{H} = \mathcal{M} H$$

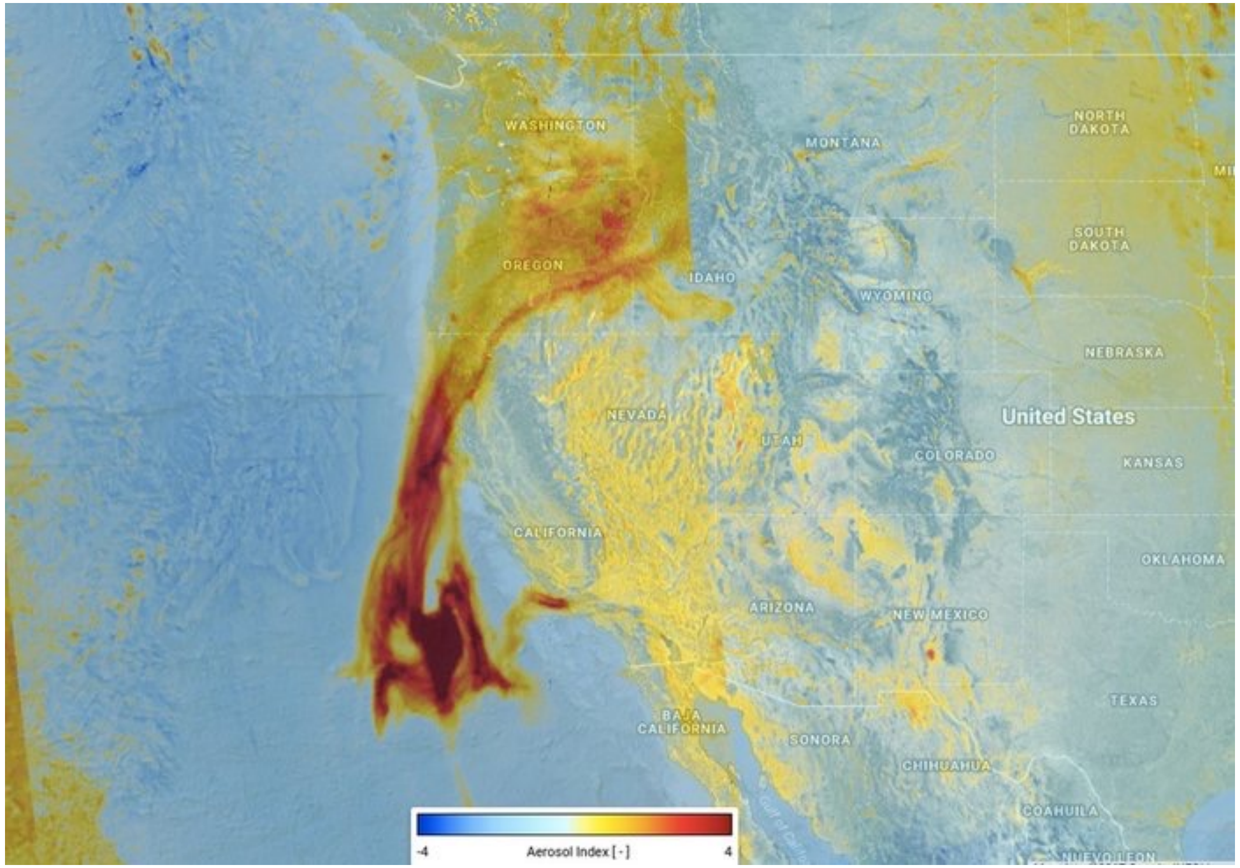
$\mathcal{M}$ Model integration

H Observation operator

Some examples from TropOMI



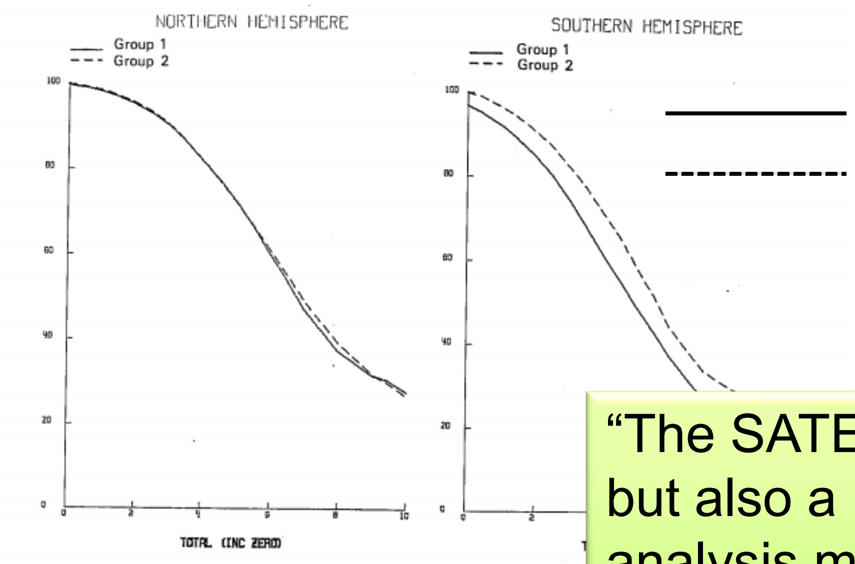
NO_2 detection of anthropogenic sources



Aerosol from fires plumes (US)

Contains modified Copernicus Sentinel data (2017), processed by KNMI

Use of retrievals in NWP – the 80s



——— No satellite data

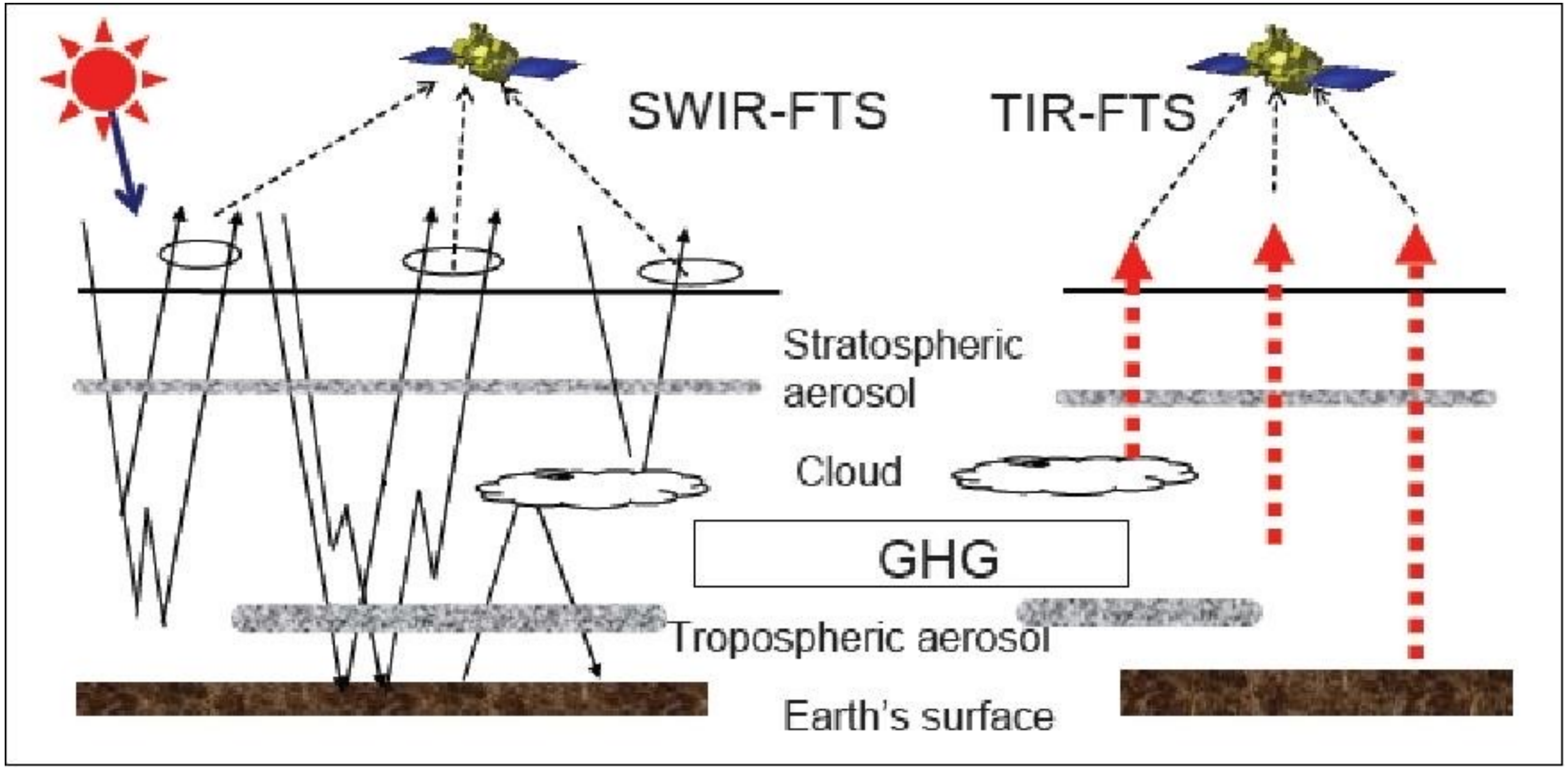
------------ L2 satellite data

Kelly and Pailleux, 1988

"The SATEMs contain some good information, but also a lot of noise and a lot of bad data. The analysis manages to maintain a large part of the good information, but is also affected by the poor quality data."

Assimilating temperature and water vapour satellite retrievals caused severe problems. Only after switch to radiance assimilation the real value of satellites was seen.

Assimilating L1 radiances for composition



Credit: JAXA

Radiance assimilation in UltraViolet, Visible, and Short-Wave InfraRed is much more complicated than in Thermal InfraRed or MicroWave.

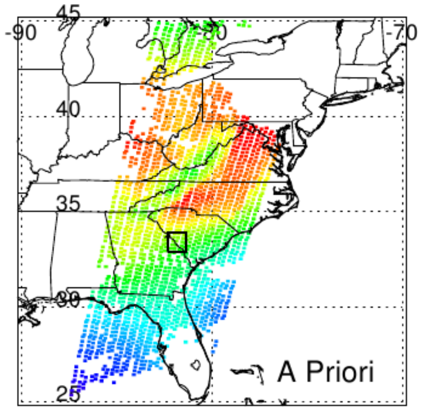
Implementing fast but accurate radiative transfer models in an operational time-critical 4D-Var system is therefore challenging.

The retrieval equation

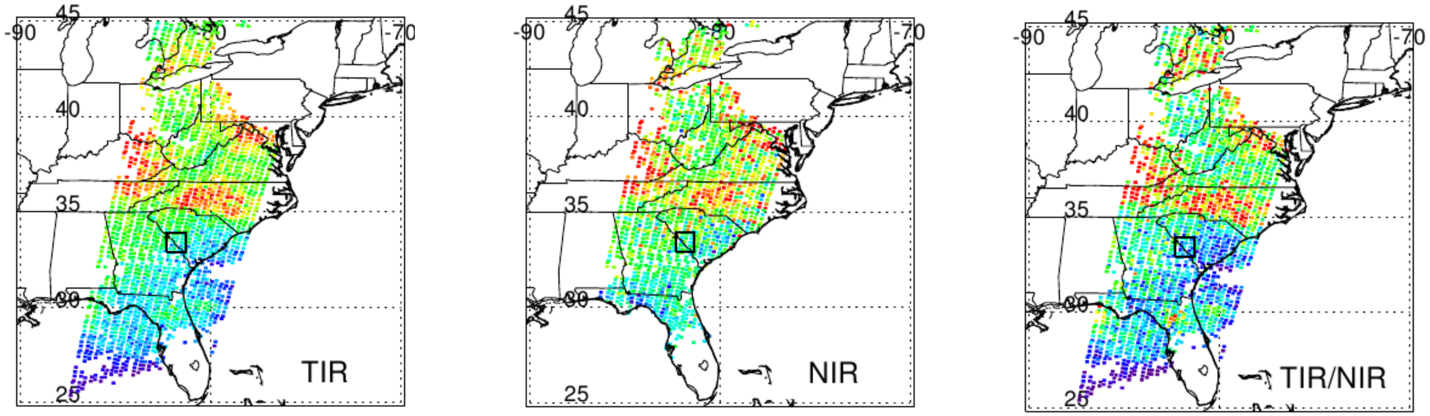
$$\hat{x} = x_r^b + \mathbf{A}(x - x_r^b) + \boldsymbol{\varepsilon}$$

The averaging kernel **A** is the sensitivity (in that case on the vertical) to the true state.
It is essential to take this into account.

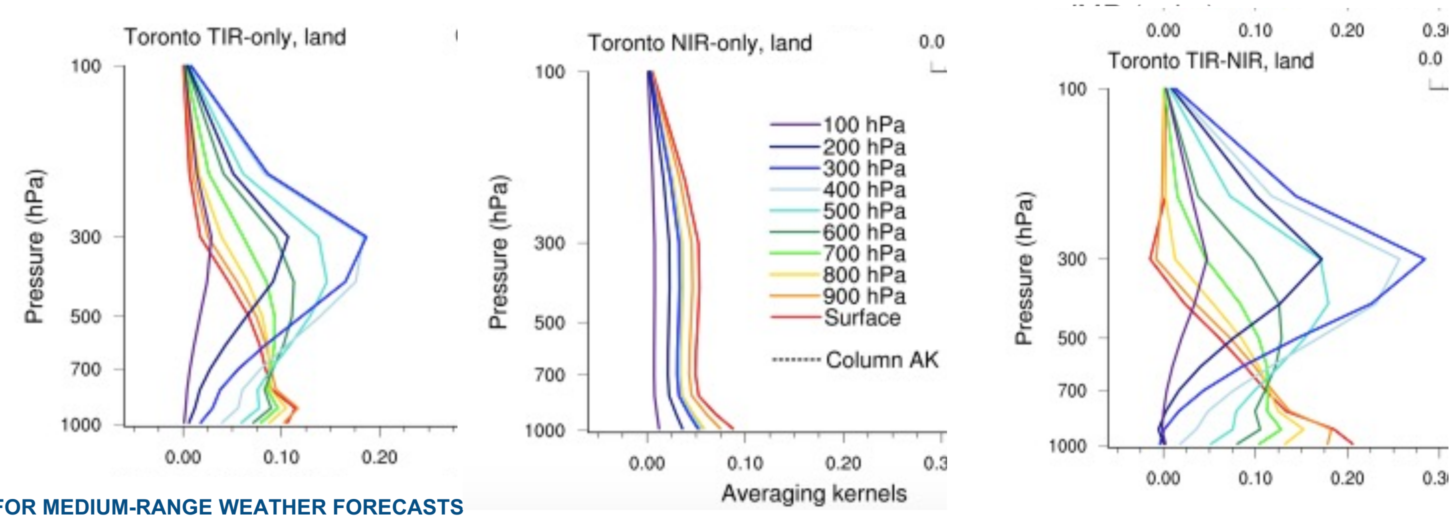
x_a



$\hat{x}$



$\mathbf{A}$



Assimilating retrievals: Column retrieval example

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

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

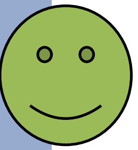
Without averaging kernels in observation operator

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

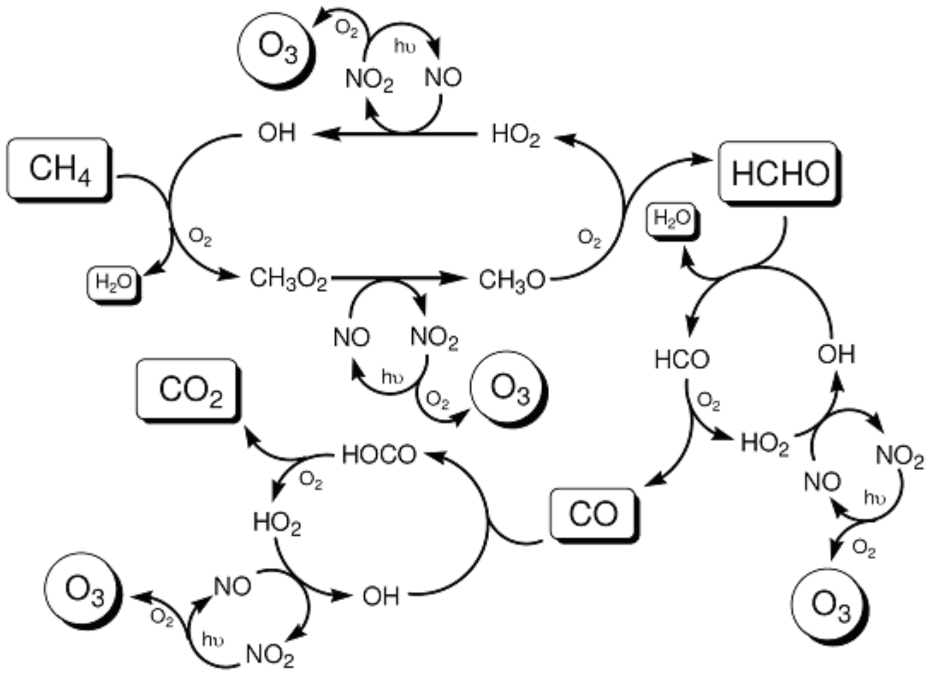
We remove the influence of the a-priori profile if we use the averaging kernel to sample the model profile according to the assumptions made in the retrieval.

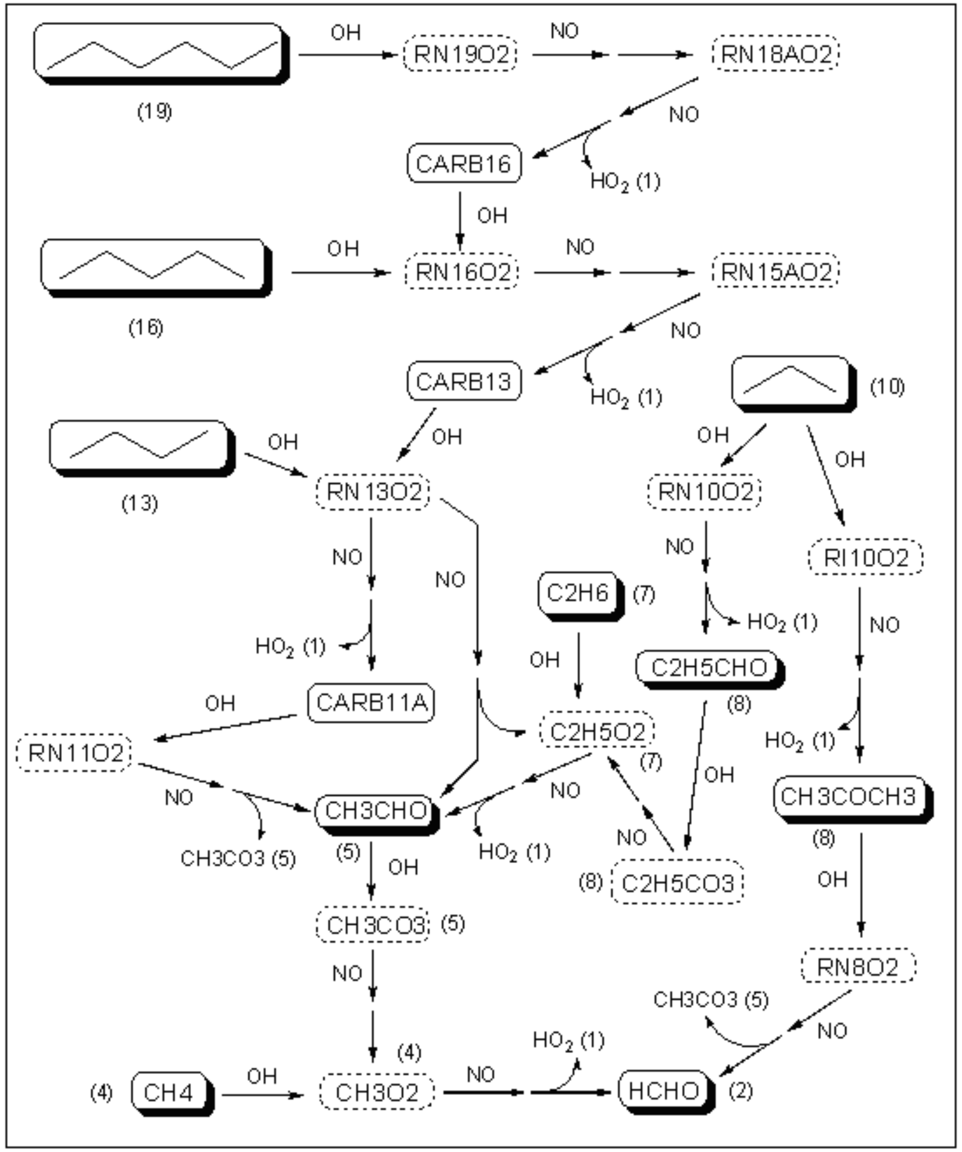
Issues

- 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

Dealing with many (reactive) atmospheric species

Atmospheric Chemistry

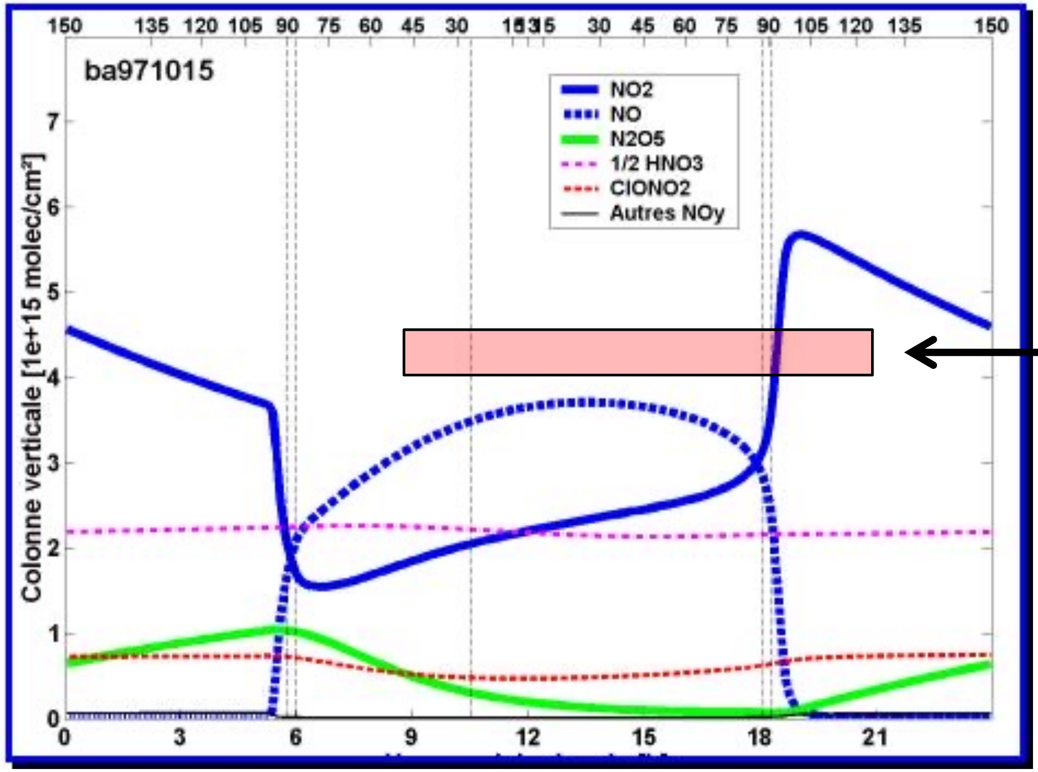




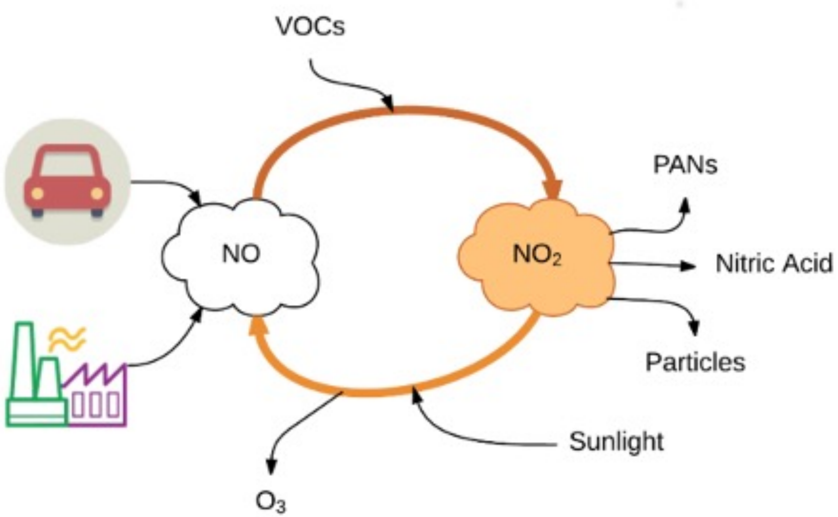
Complexity can go very far… with master mechanisms of about 10000 variables

Usually, it is costly to model and simplifications are mandatory to run an operational forecasting system with only around 50 variables.

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.

Include simple chemistry in TL/AD

Photochemical equilibrium:

- $NO + O_3$ -> NO_2
- NO_2 + hv -> $NO + O_3$

Loss term for NOx:

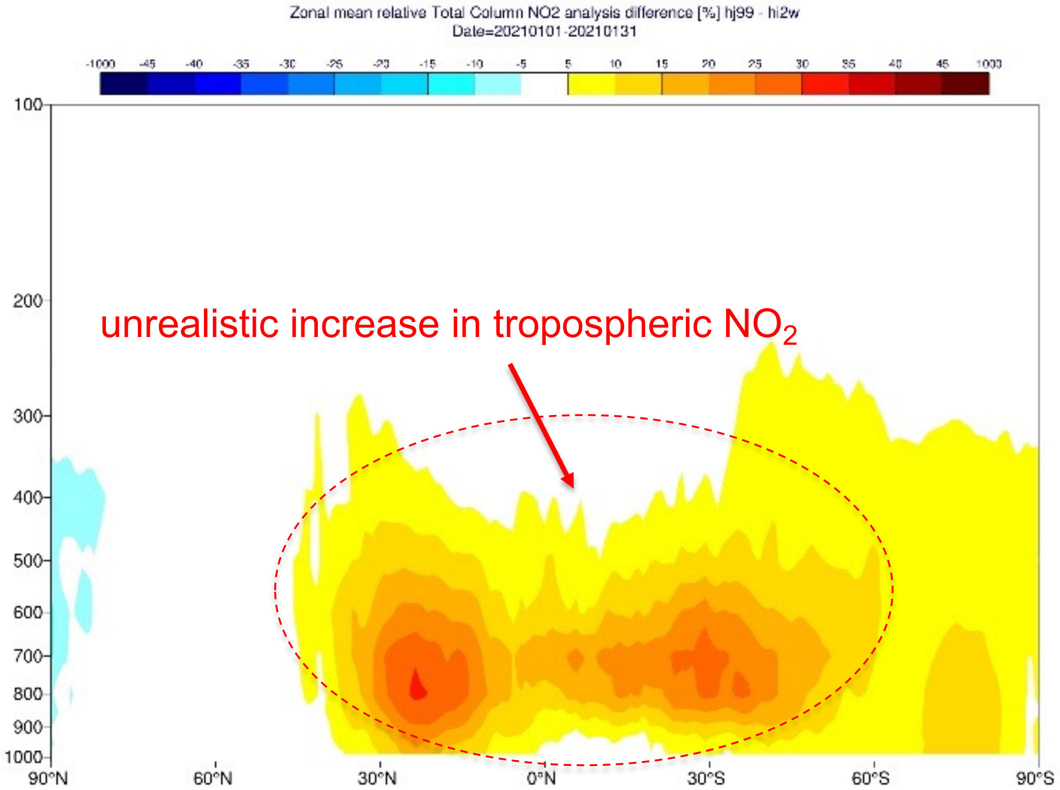
- NO_2 + OH -> HNO_3

- 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).

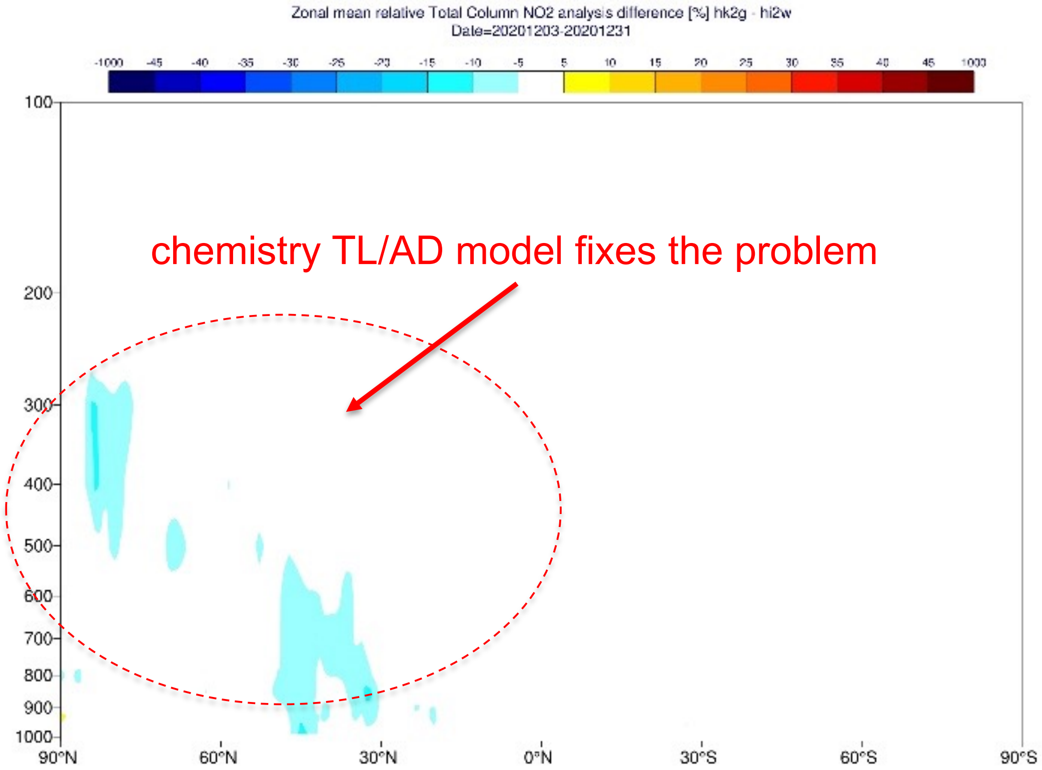
Simplified chemistry TL/AD

Impact of TROPOMI NO_2 assimilation

No chem - CTRL



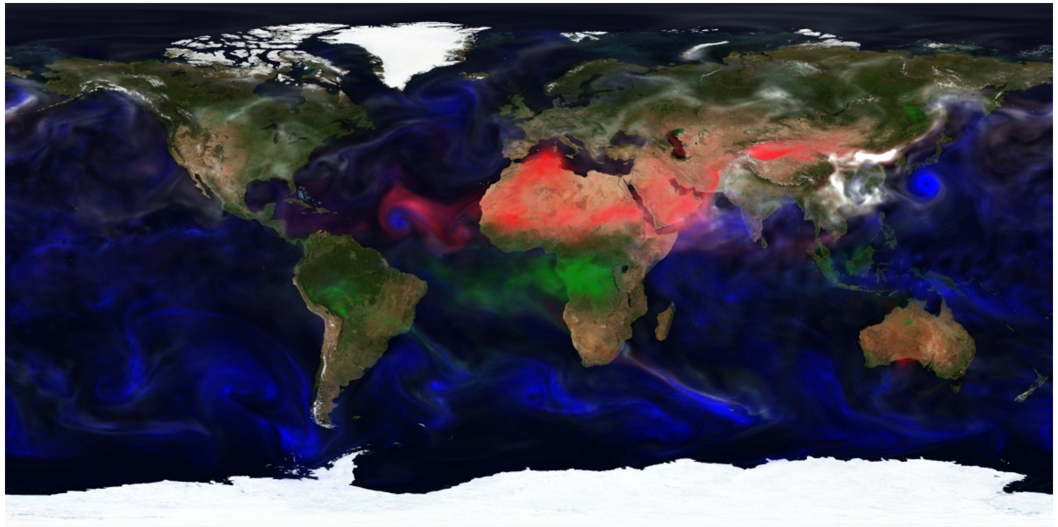
Simplified chem - CTRL

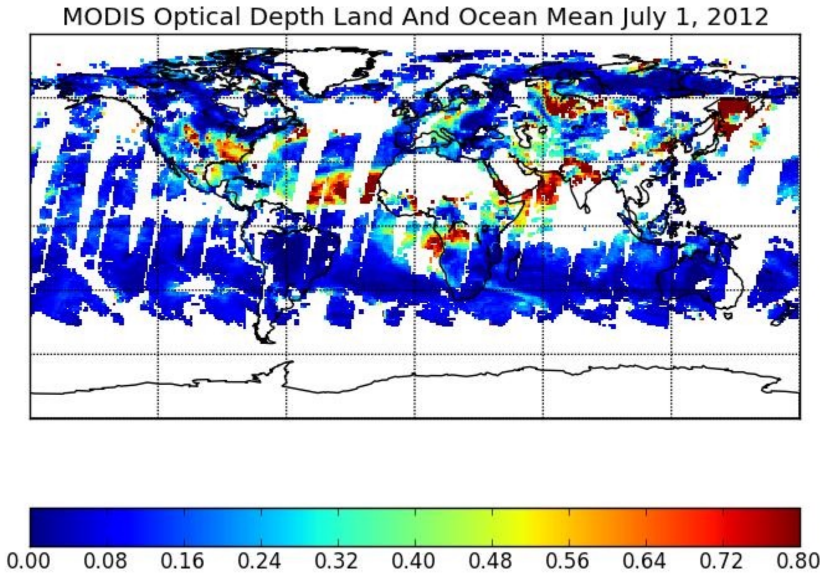


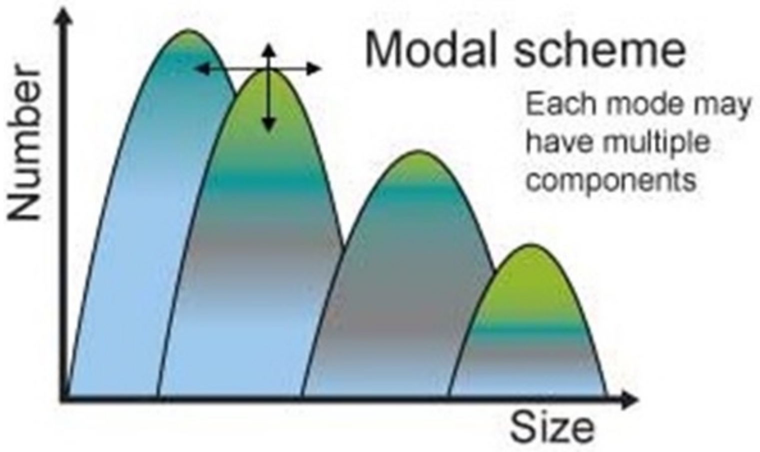
3-31/12/2020

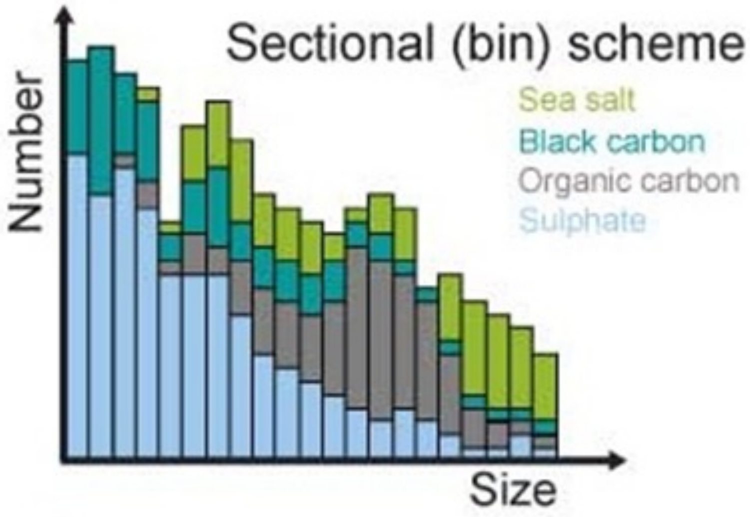
Relative zonal mean differences [%]

Aerosol – prime example of ill-observed system









Aerosol analysis

- CAMS aerosol model has 14 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

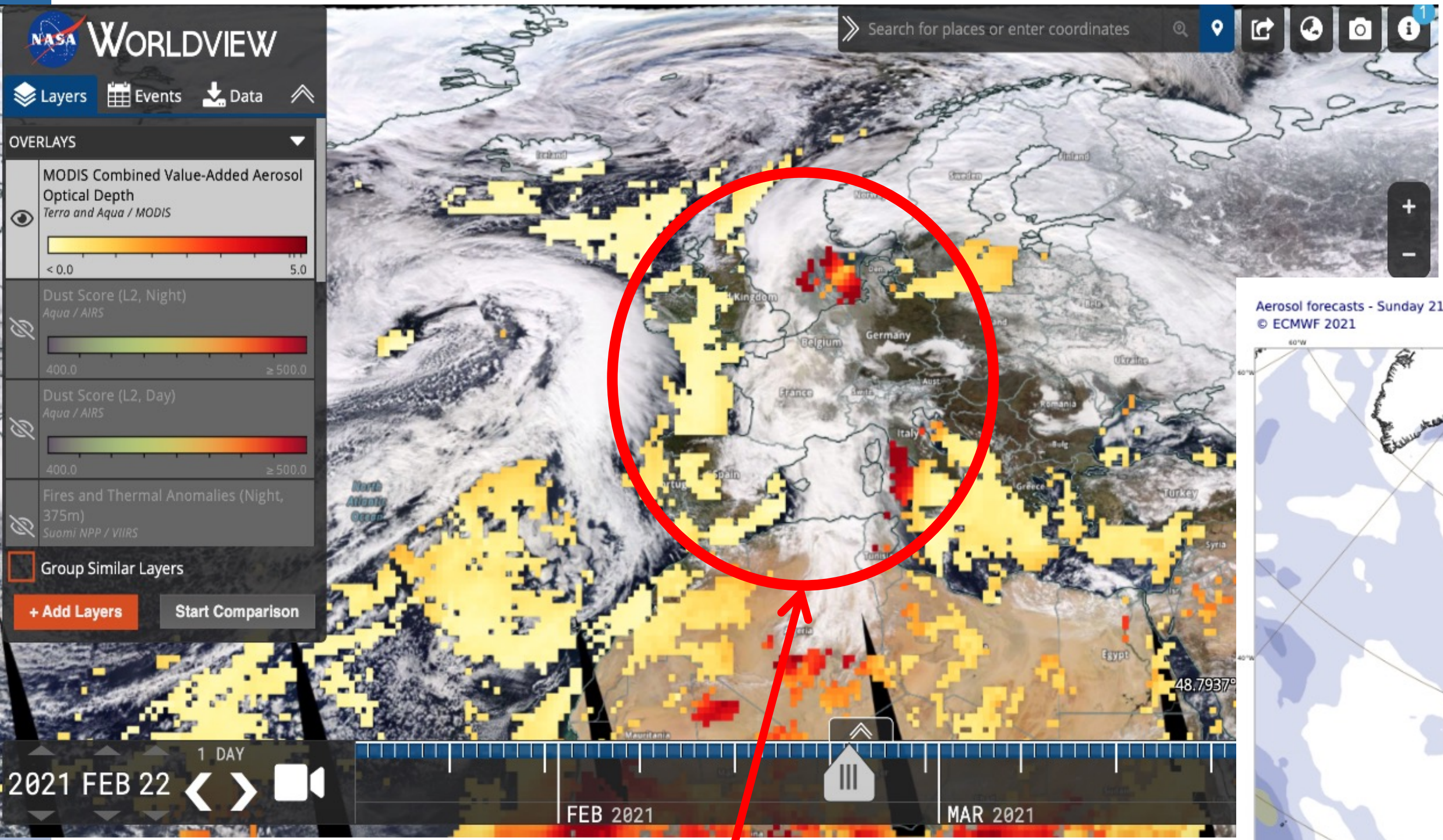
- Assimilated observations are Aerosol Optical Depth (AOD) at 550 nm from various satellite sensors. AOD is a measure of the total aerosol amount in a column.

- 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.

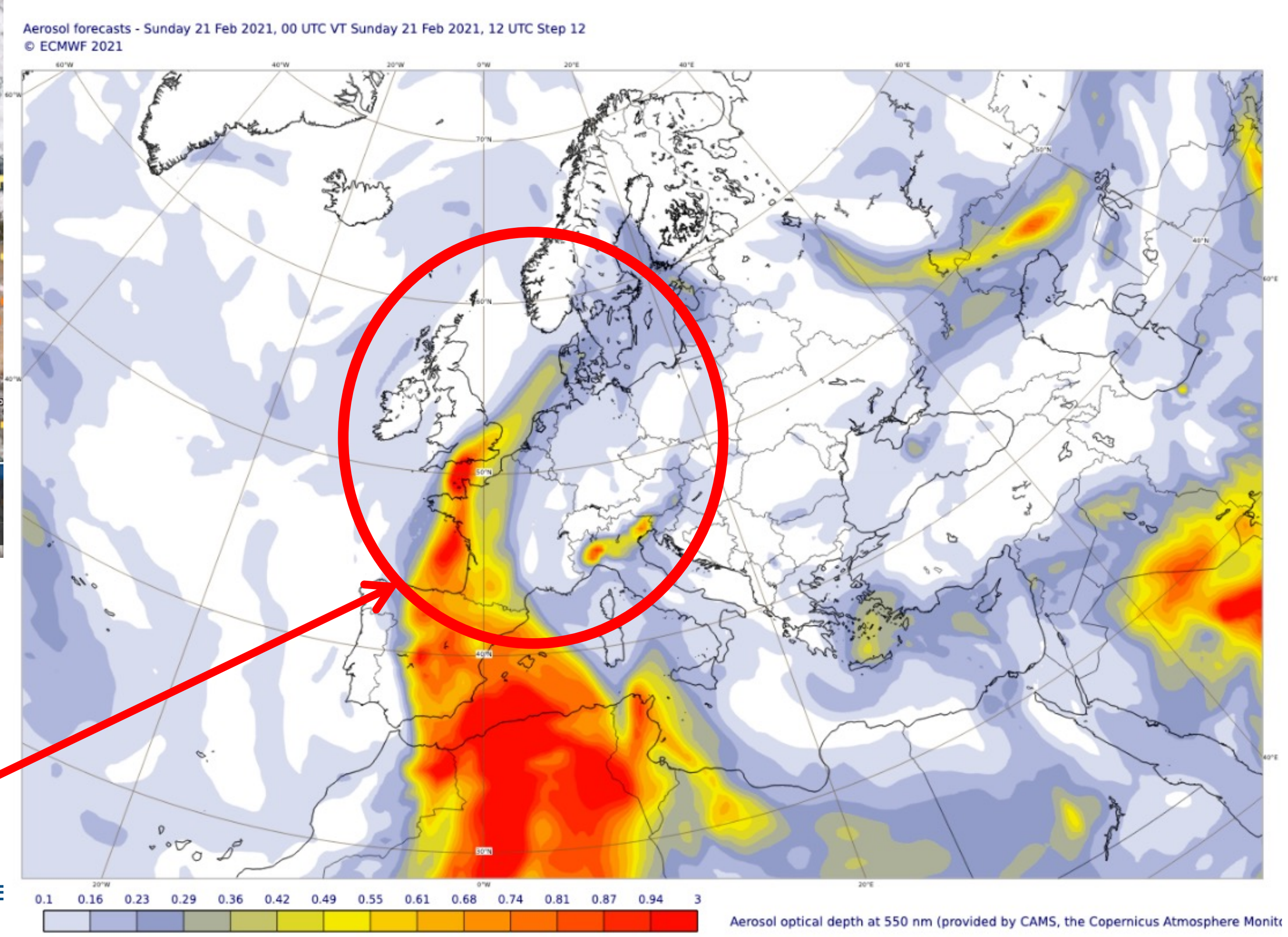
- The repartitioning of the total aerosol mixing ratio increment into the different bins is difficult

Dust storm February 2021



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

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

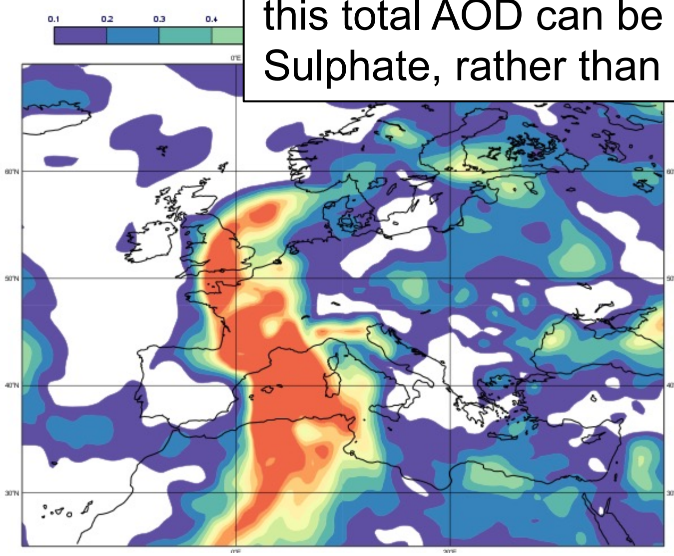


The CAMS forecast does a good job of forecasting the AOD plume from Africa over Northern Europe

ECMWF EUROPEAN CENTRE FOR MEDIUM-RANGE WEATHER FORE

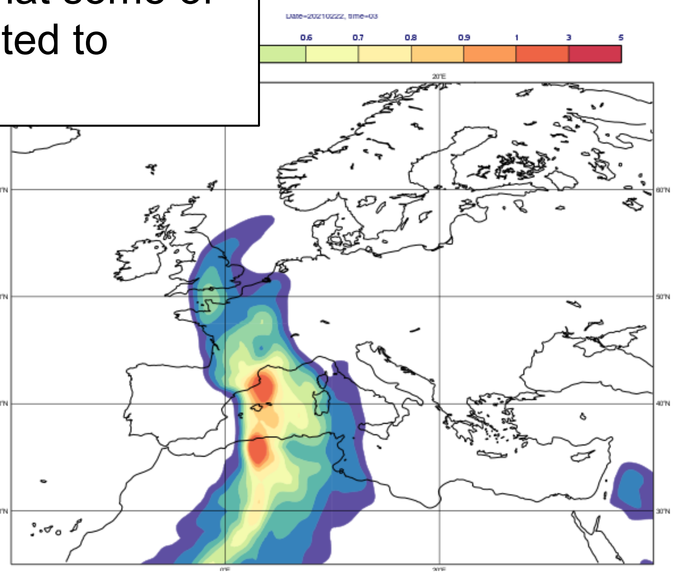
Dust test case February 2021

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

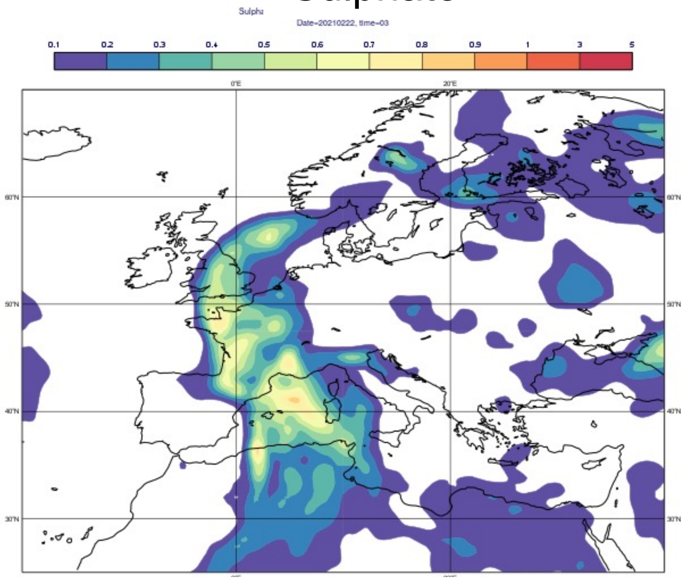


Total AOD at 550nm: 20210222 03hr

Dust

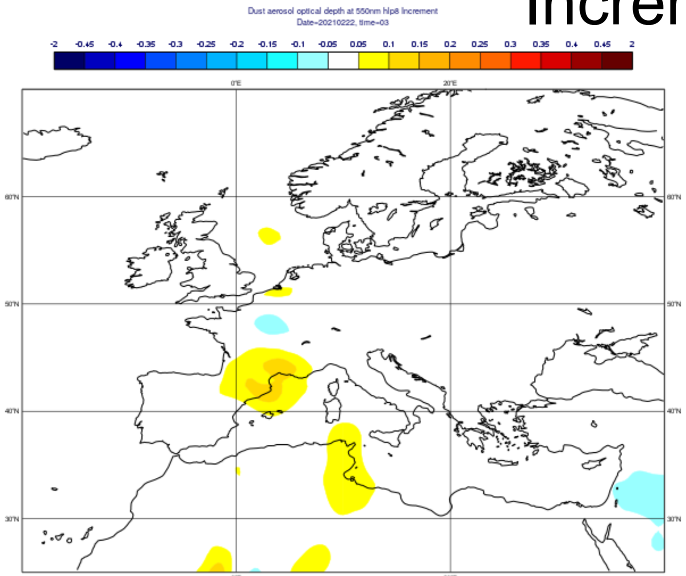


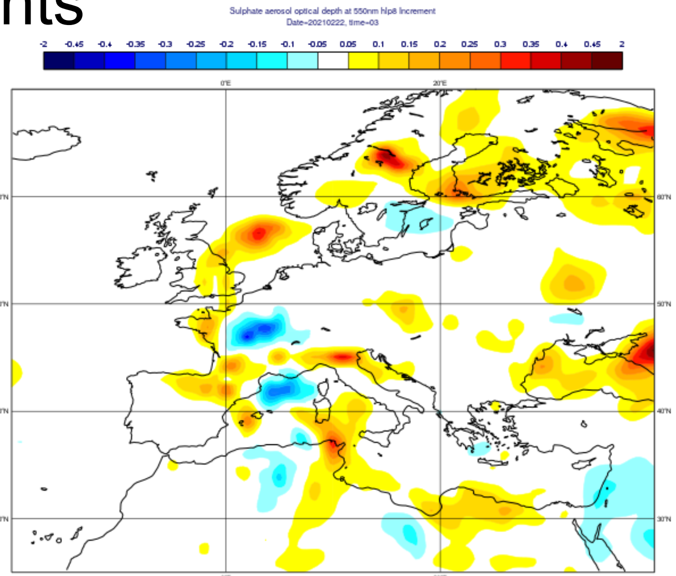
Sulphate



AOD at 550nm

Increments





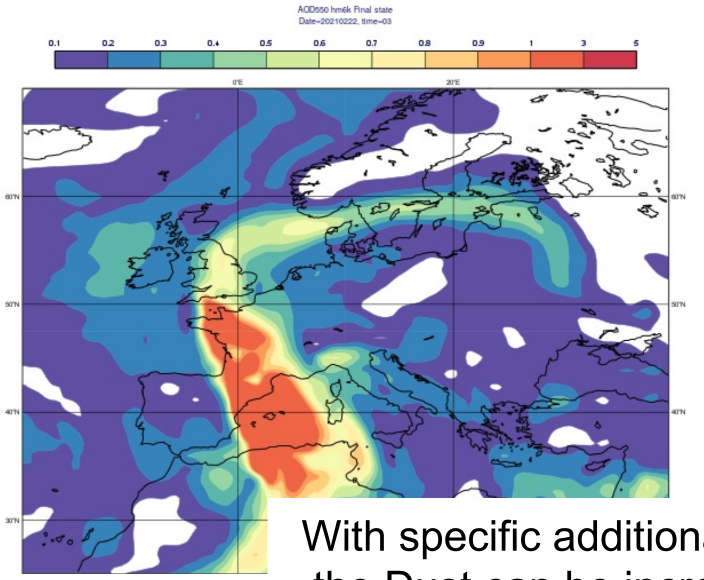
AOD incr at 550nm

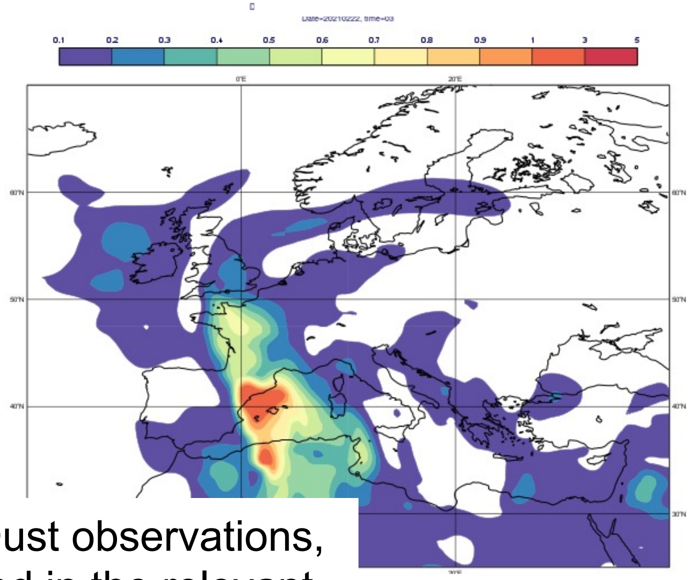
- AOD increments are attributed to the different species according to their proportion in the nonlinear forecast.
- If there is no dust in the forecast in a specific location then the increment will be given to whatever species are there – in this case Sulphate

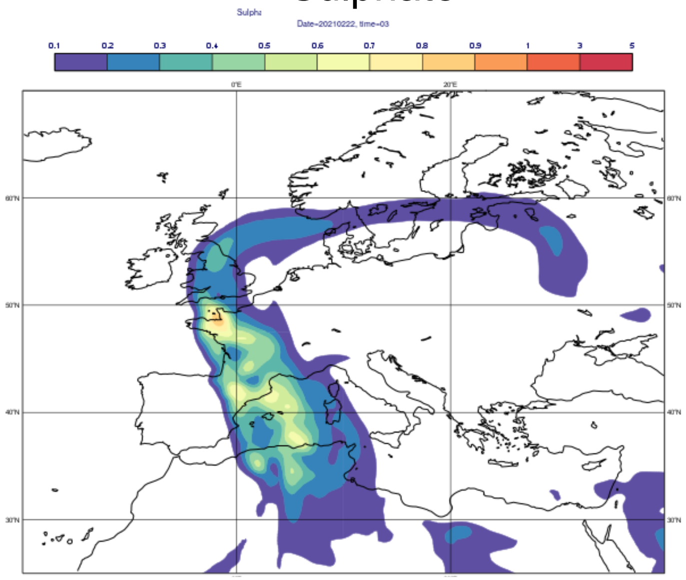
Dust test case February 2021

Dust

Sulphate

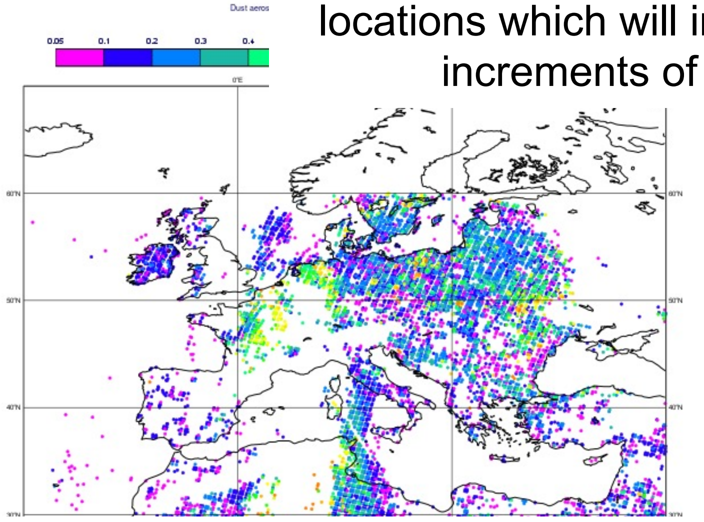




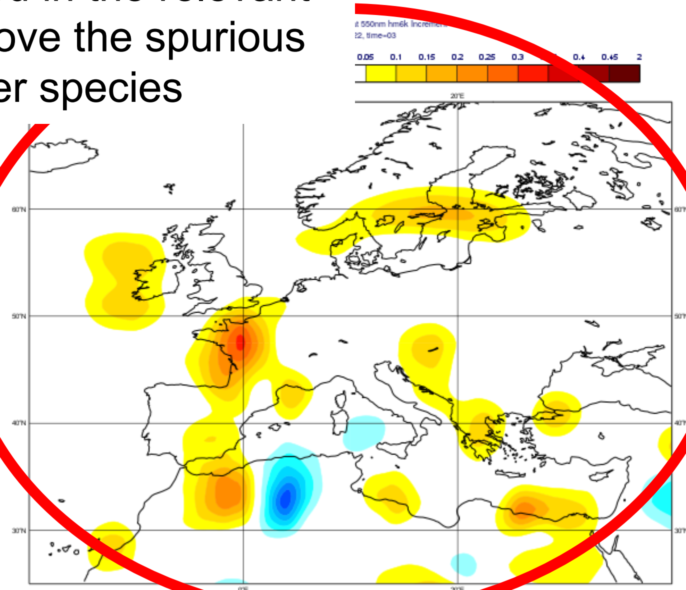


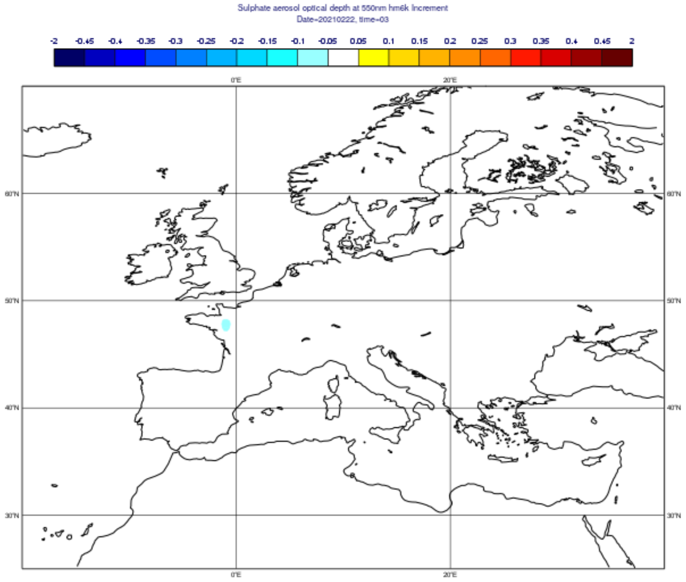
AOD at 550nm

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



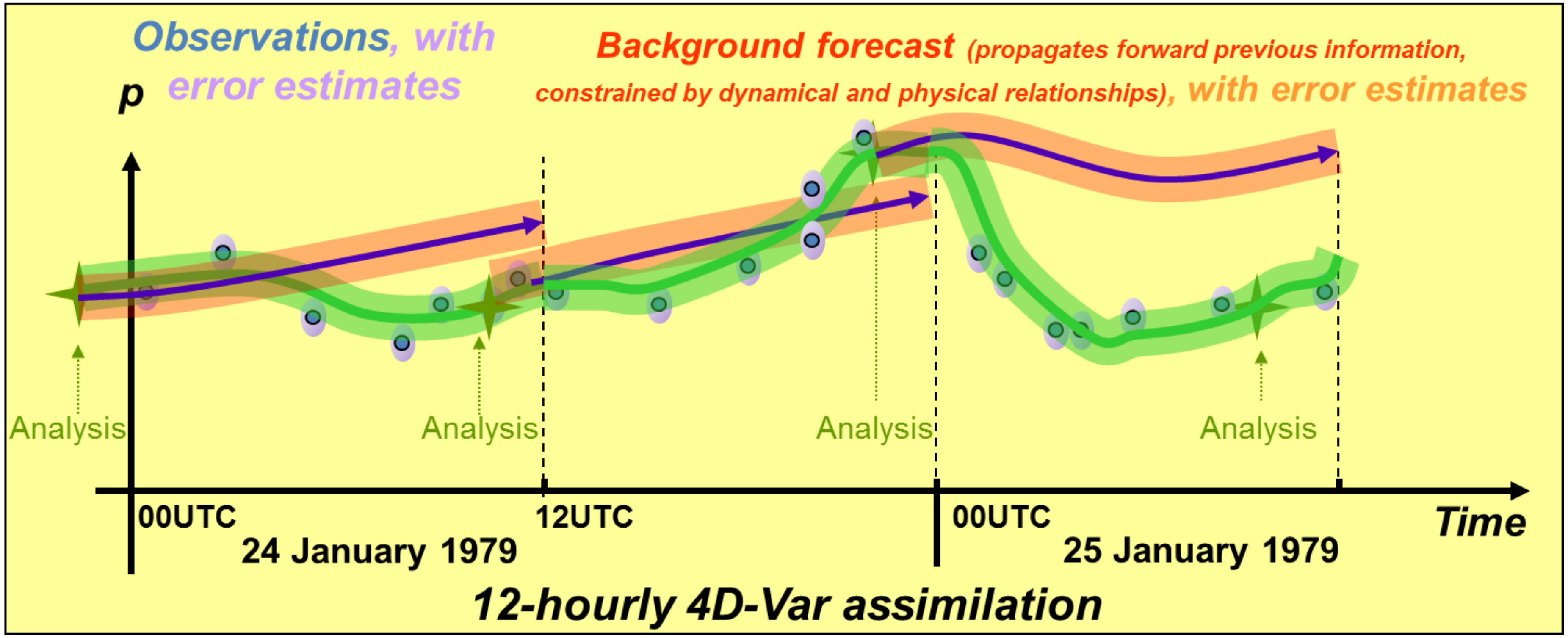


AOD incr at 550nm

Initial versus boundary values:

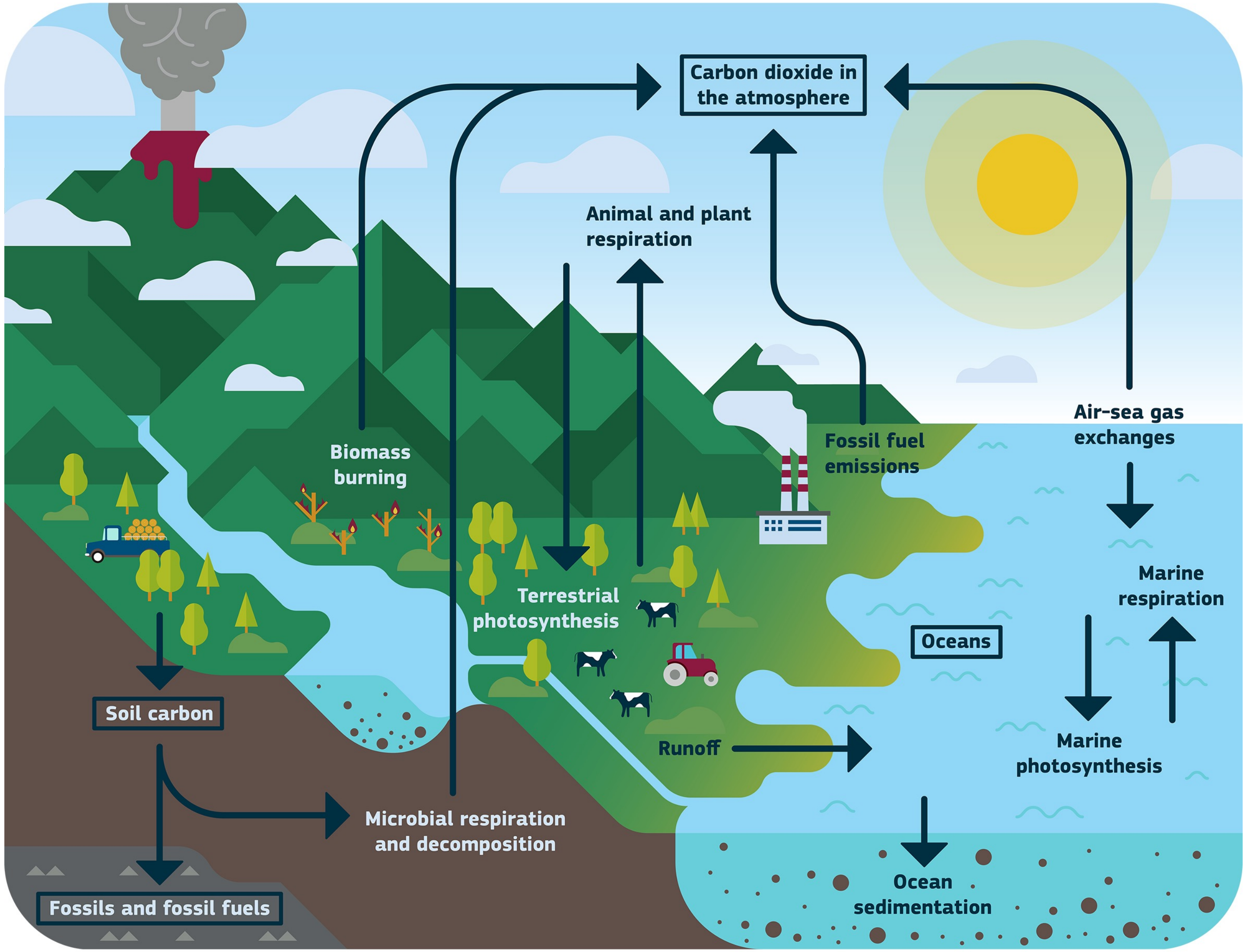
the surface fluxes

4D-Var



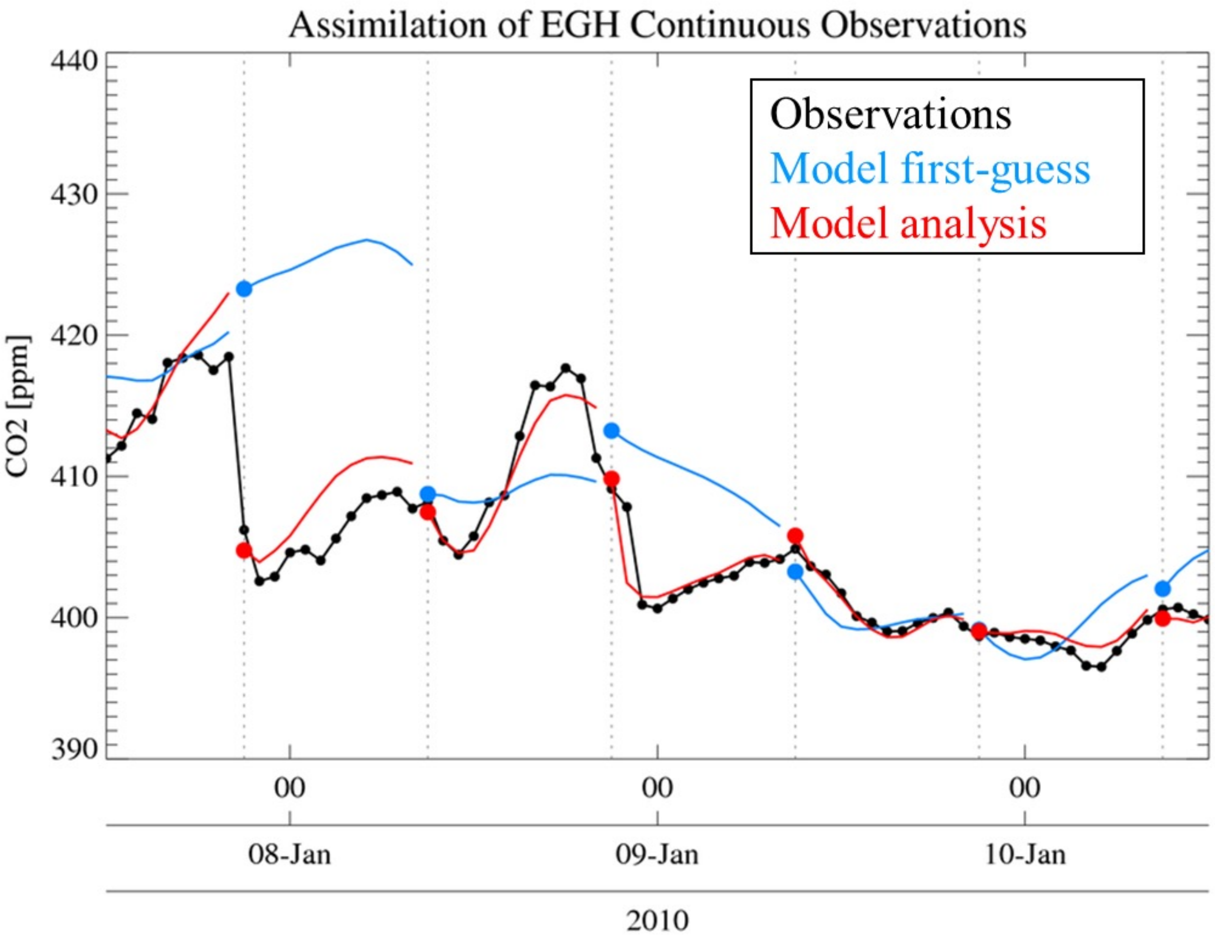
NWP 4D-Var is mostly defined as an initial value problem. Only initial conditions are changed and model error is relatively small.

CO_2 as an example – a boundary condition problem



Boundary condition problem – CO_2

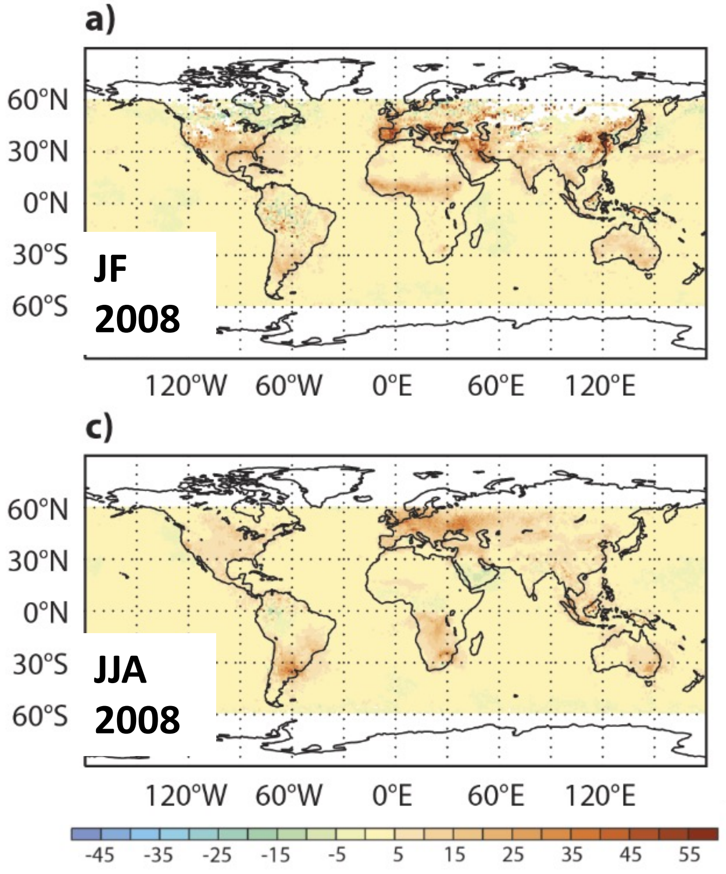
Example: Assimilation of surface observations



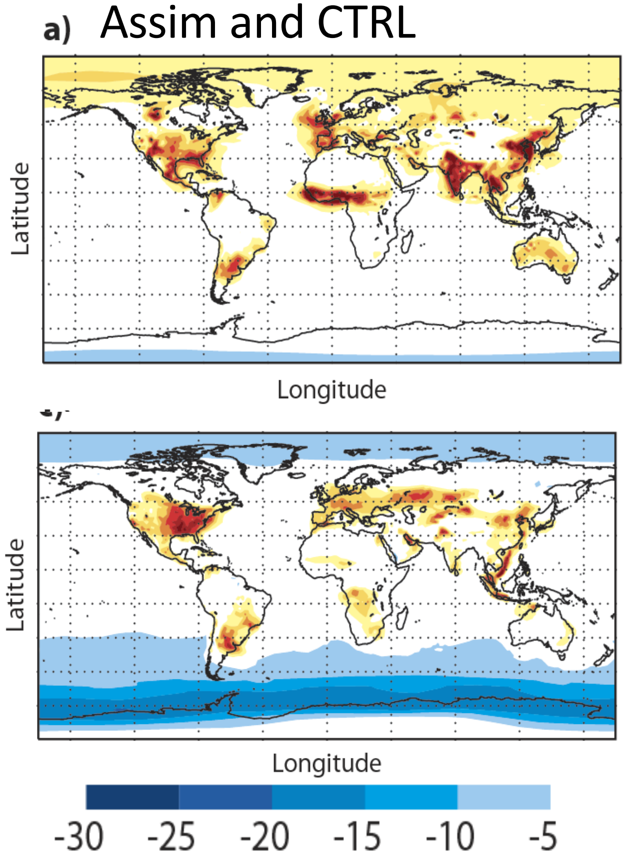
By only adjusting the initial conditions, the forecast can drift very quickly from the actual observations.

Short-lived memory of NO_2 assimilation

OMI NO_2 analysis increment [%]



Differences between Assim and CTRL

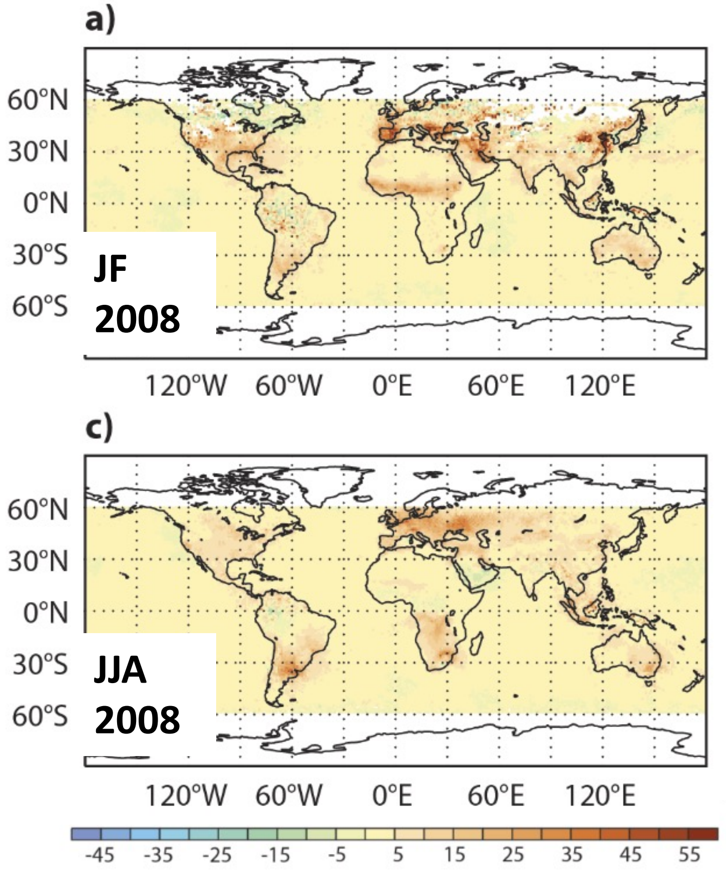


- Large positive increments from OMI NO_2 assim
- Large differences between analyses of ASSIM and CTRL

Inness et al. (2015, ACP)

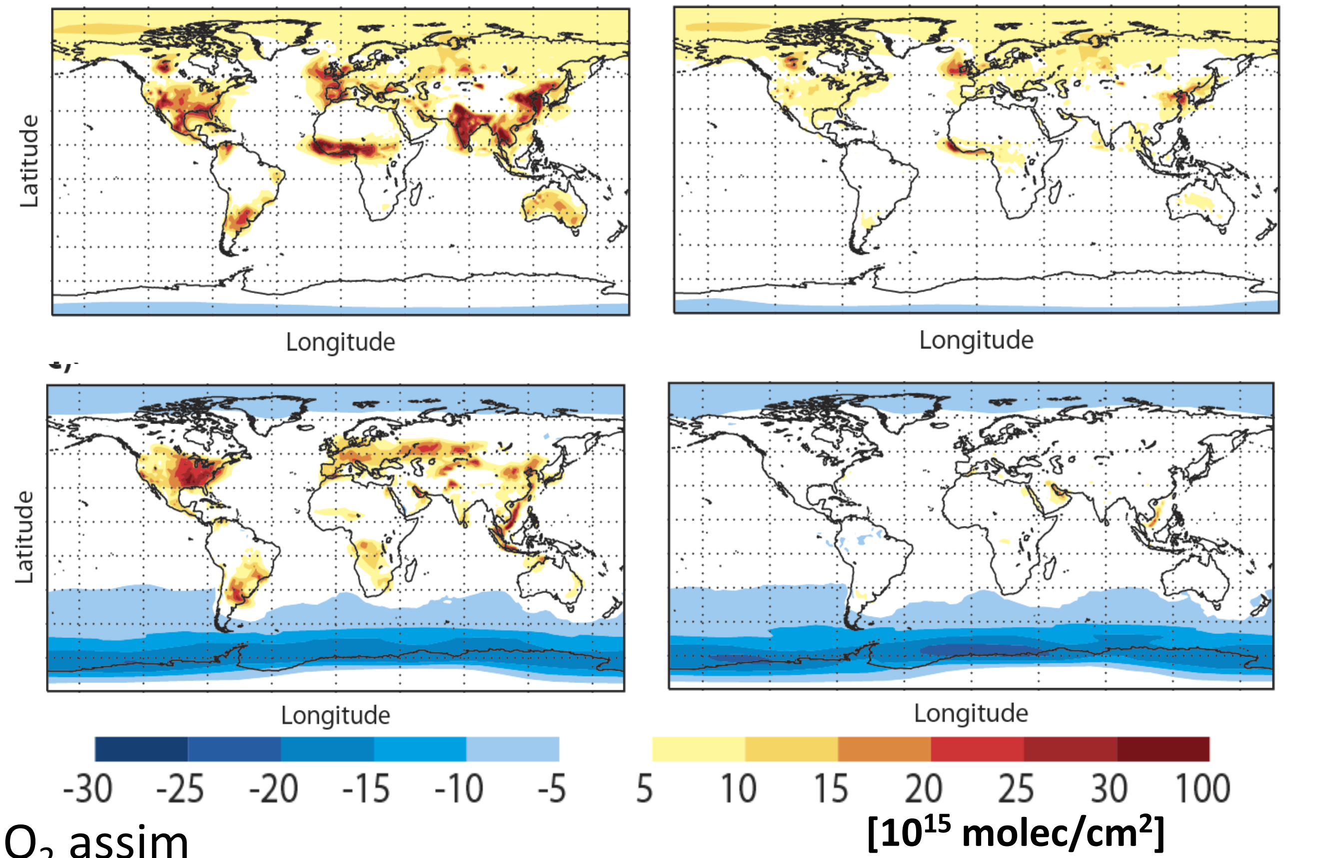
Short-lived memory of NO_2 assimilation

OMI NO_2 analysis increment [%]



Differences between
a) Assim and CTRL

Difference between 12h forecasts from ASSIM and CTRL

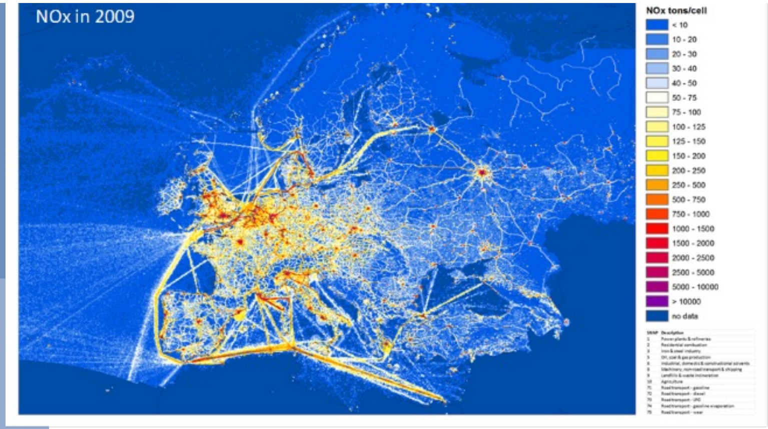


- Large positive increments from OMI NO_2 assim
- Large differences between analyses of ASSIM and CTRL
- Impact is lost during subsequent 12h forecast
- Constraining emissions (in addition of IC) would give a better initial state and persistence of forecast improvements throughout the DA window

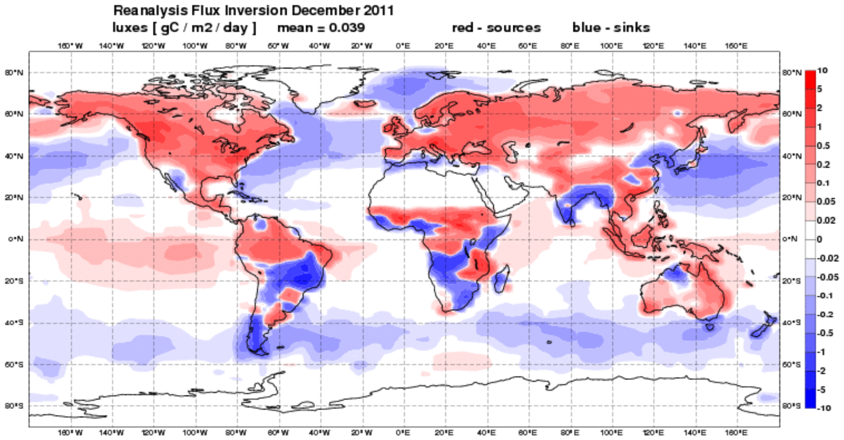
Inness et al. (2015, ACP)

Need for very accurate emission data sets

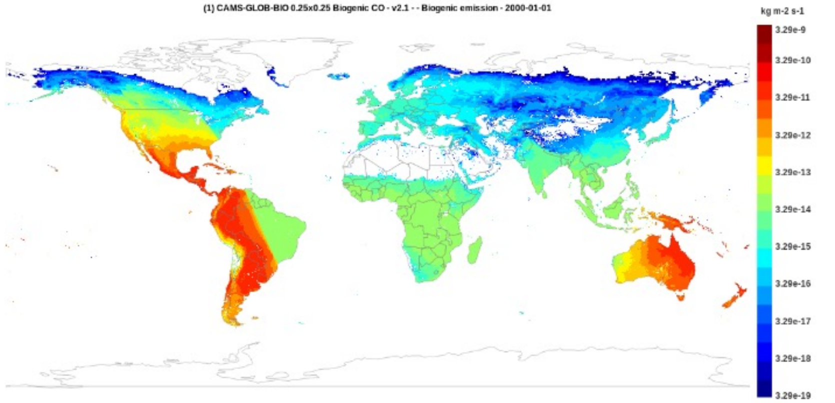
TNO European anthropogenic NOx emissions



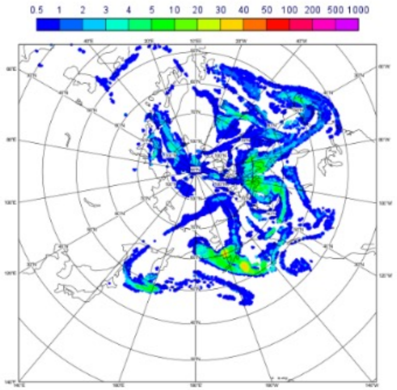
CO_2 fluxes



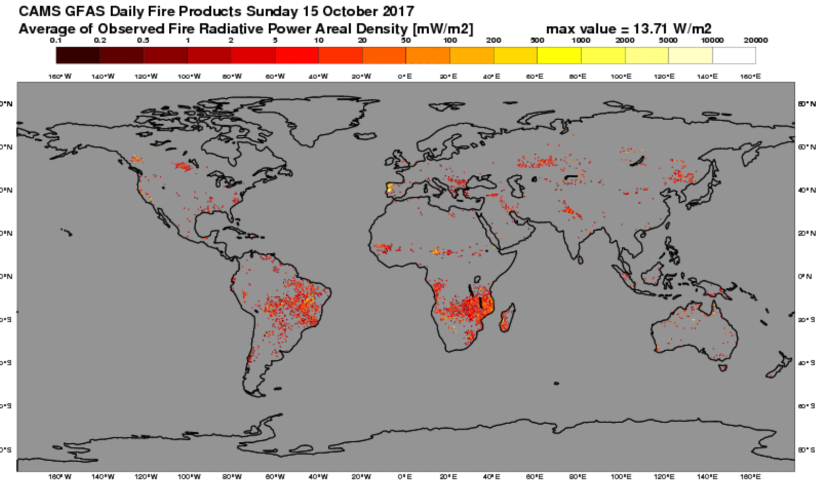
CAMS_GLOB biogenic CO emissions



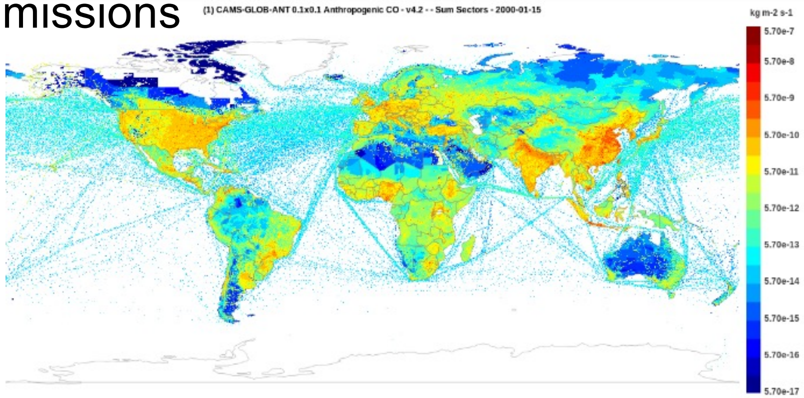
Volcanic SO_2



Biomass burning, 15 October 2017



CAMS_GLOB anthropogenic emissions

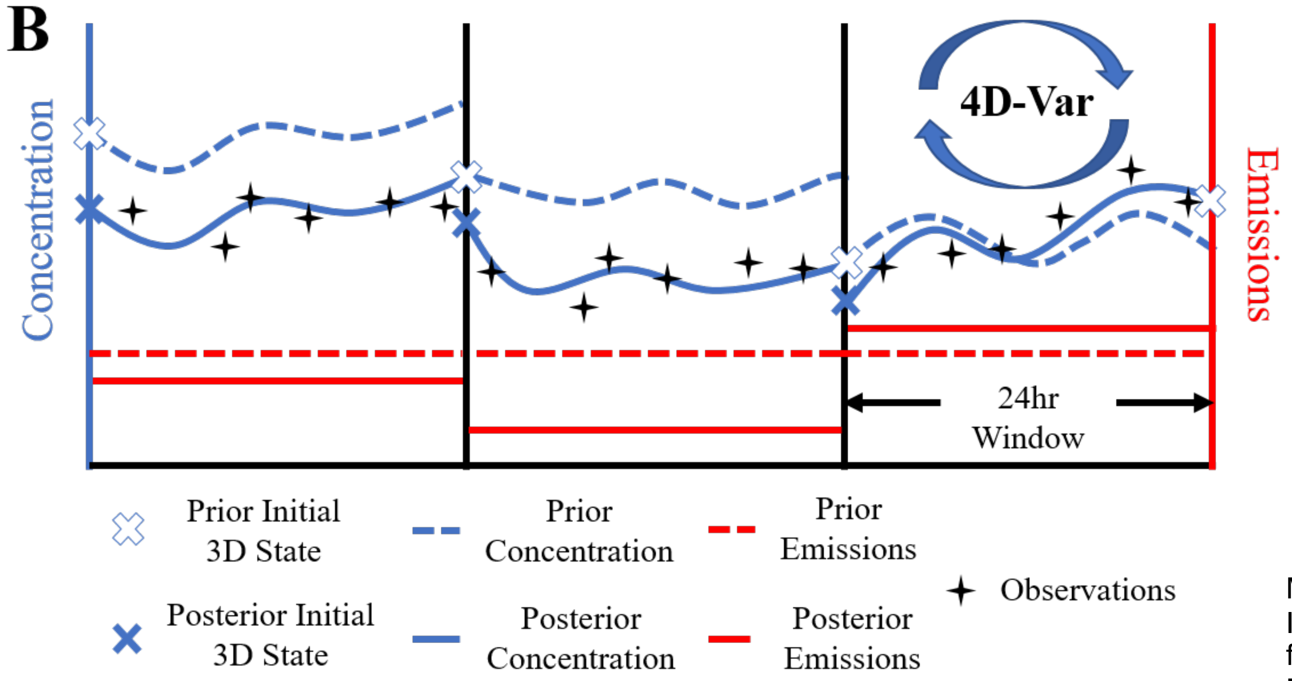


Emission Estimates

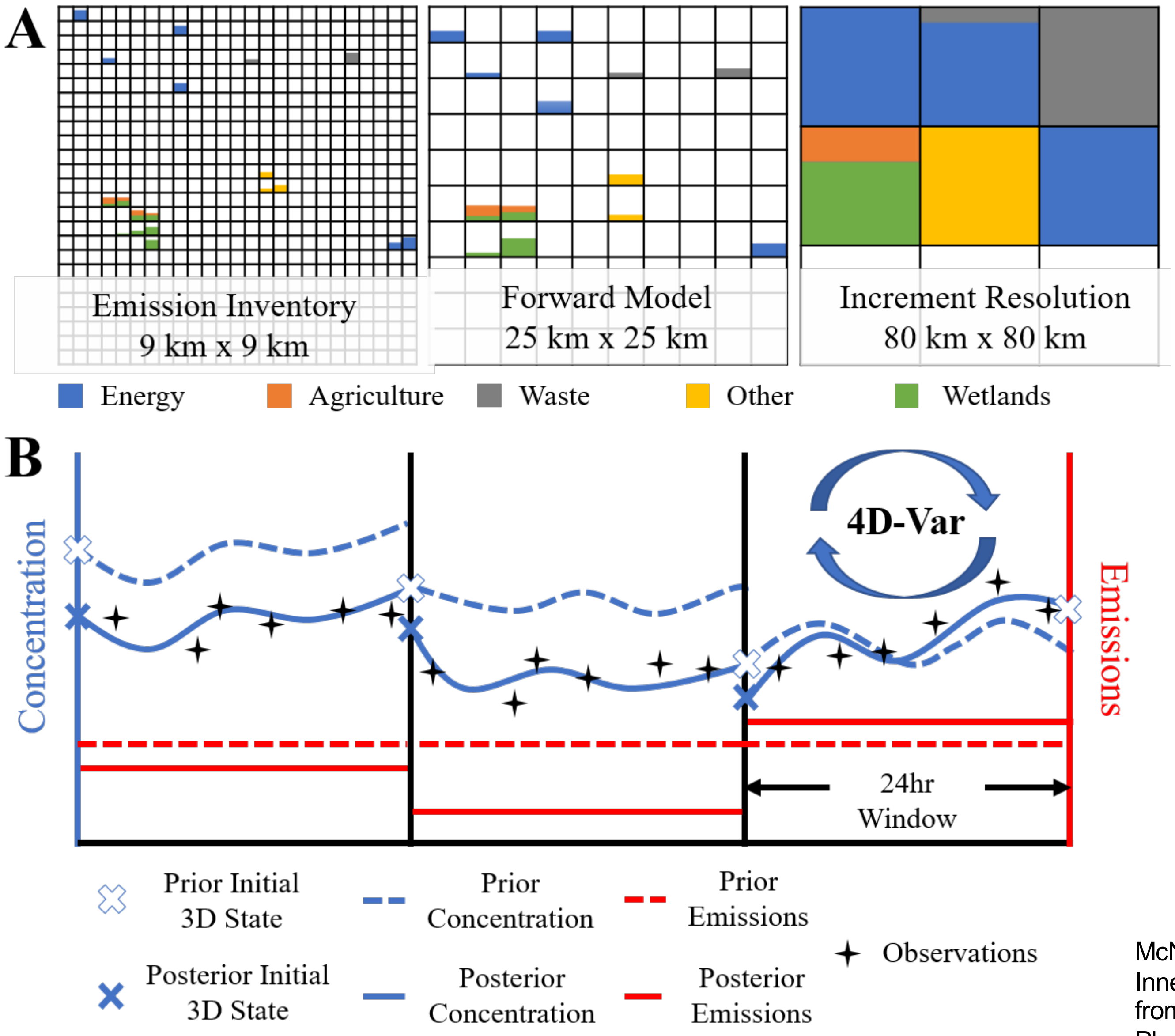
- Emissions are one of the major uncertainties in composition modeling (can not be measured directly)
- The compilation of emissions inventories is a labour-intensive task based on a wide variety of socio-economic and land use data
- Some emissions can be “modeled” based on wind (dust and sea salt aerosol) 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

How to improve?

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



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.



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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.

Joint state/emissions 4D-var inversion system

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

State control vector

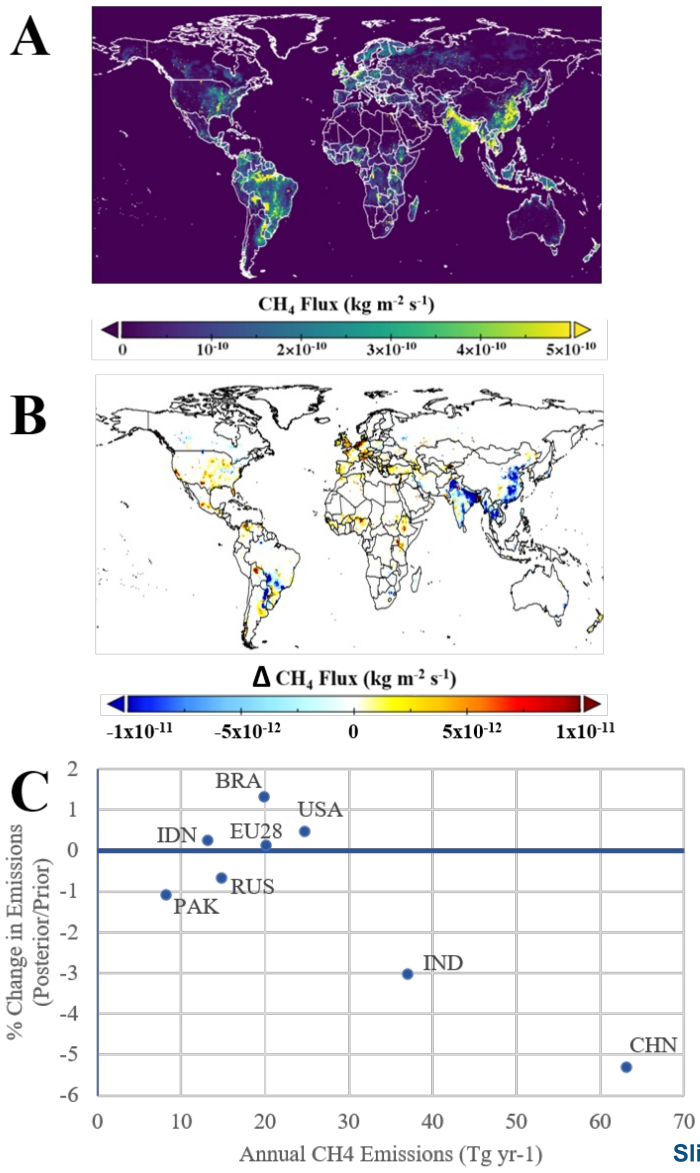
Parameter (e.g. scaling factors)

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

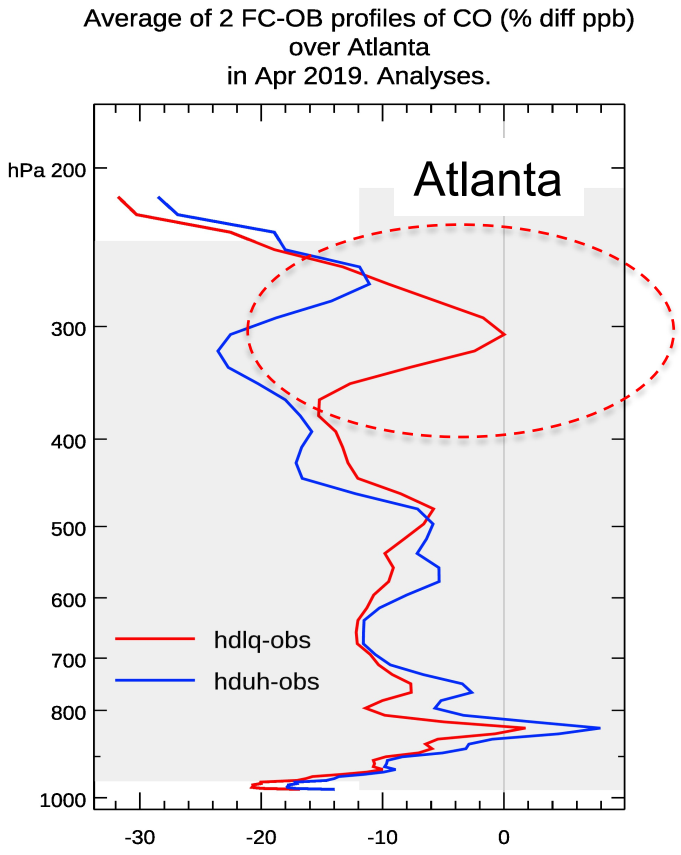
- Joint optimisation of emissions and initial conditions
- Optimized emissions for e.g., CO_2, CH_4, CO, NO & NO_2
- TL/AD of simplified chemistry: link between NO emissions and NO_2 observations
- 2D scaling factors p applied to emission fields
- Prior error definition:
    - Global constant or 2D map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

Very active research agenda for operational DA for composition

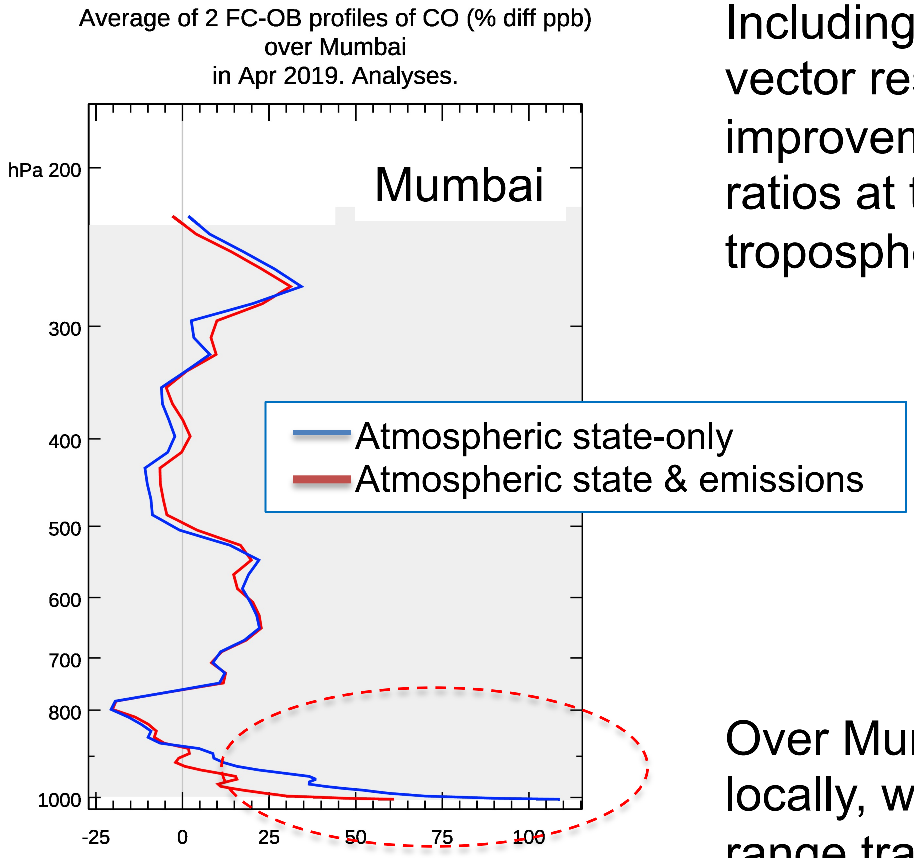
- Include emissions/fluxes in control vector
- Flux increments, correction factor, parameter estimation?
- Enough signal in a typical short assimilation window in operations (6h-12h)?
- How to propagate the information on emission constraints from window to window? No forward model.
- Full chemistry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



Constraining emissions improves the forecast



%ppb difference
(FC-OBS)



%ppb difference
(FC-OBS)

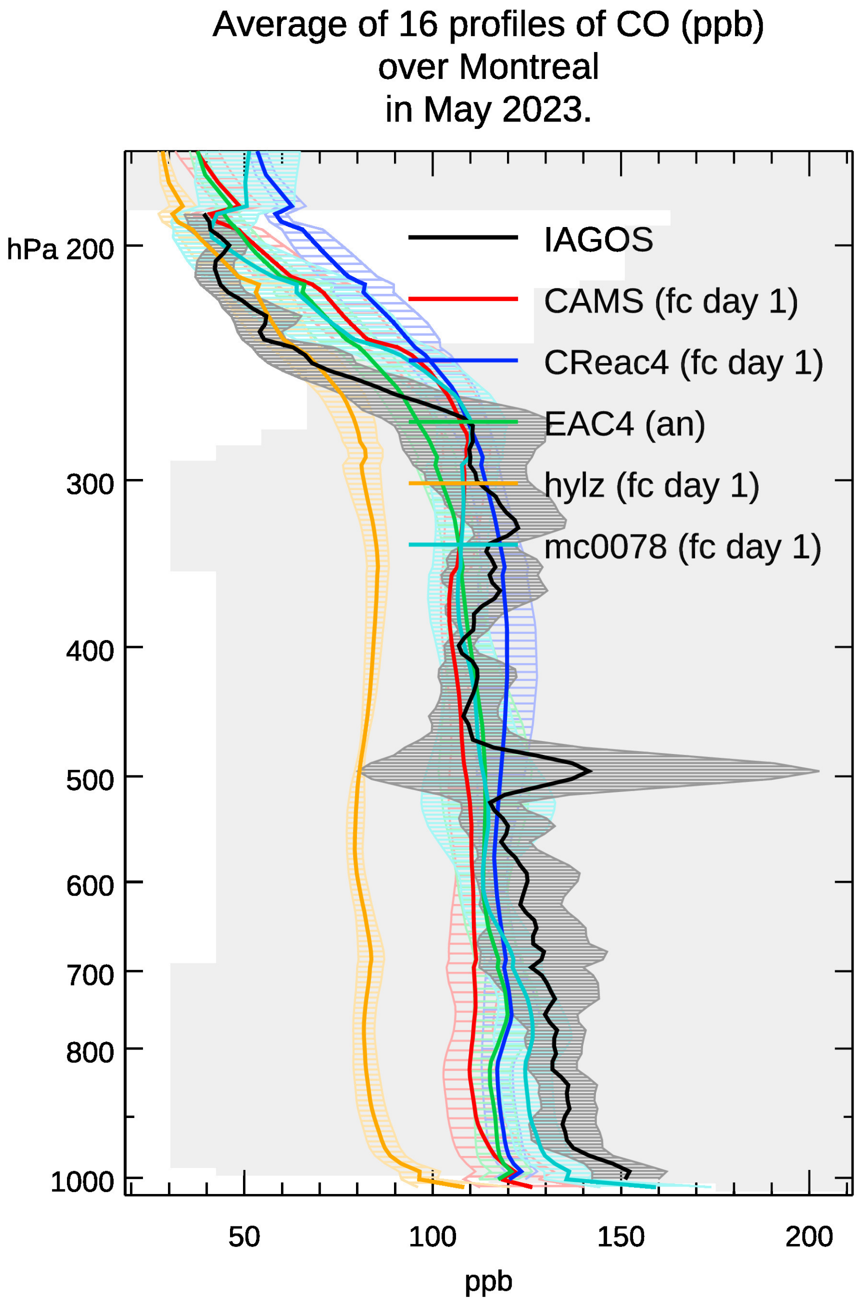
Including emissions in the DA control vector results in significant improvements in modelled CO mixing ratios at the surface and in the upper troposphere.

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

Summary in one figure

Evaluation of Carbon Monoxide in model and analysis runs against observations shows all the (potential) issues.

- Aircraft observations (black)
- Analysis with MOPITT and IASI (TIR only) (red)
- Reanalysis control run (blue)
- Reanalysis (green)
- Control run with new emissions (orange)
- Analysis with MOPITT, IASI and TROPOMI (light blue)



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