Data assimilation of atmospheric composition

Melanie Ades

ECMWF

Melanie.Ades@ecmwf.int

Contributions from: Antje Inness, Richard Engelen, Johannes Flemming, Sebastien Massart, Angela Benedetti and Alessio Bozzo

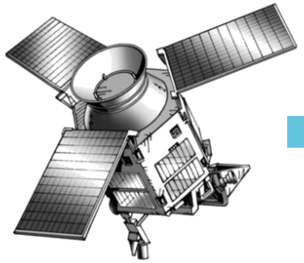
Why atmospheric composition at an operational weather centre?

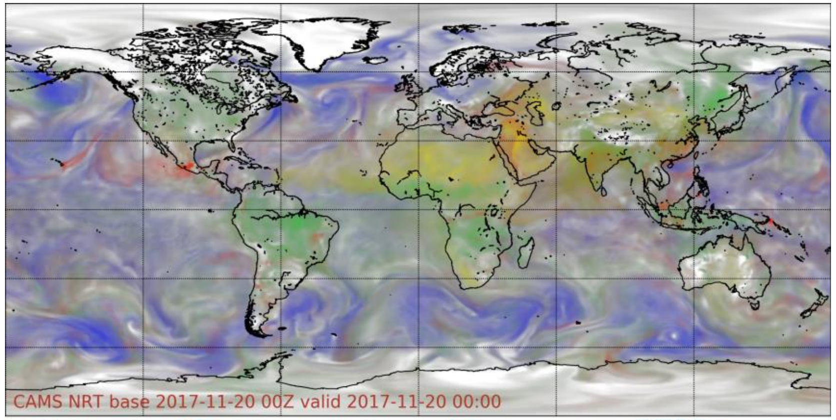
Copernicus Europe's eyes on Earth

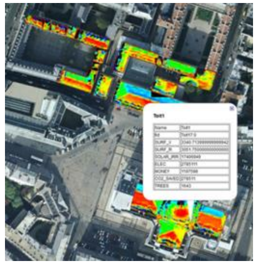
Atmosphere Monitoring Service
atmosphere.copernicus.eu

People are affected by air quality and ask for better information

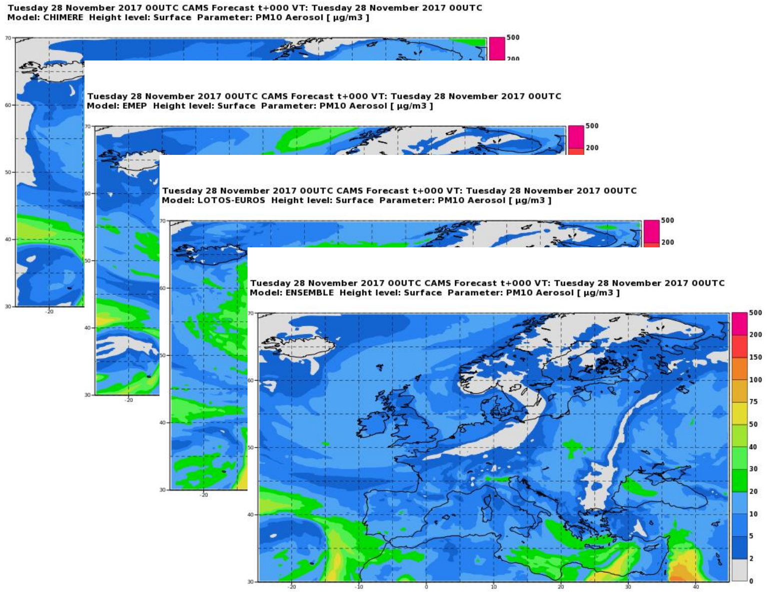
Copernicus Atmosphere Monitoring Service

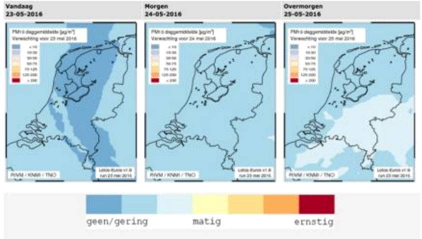






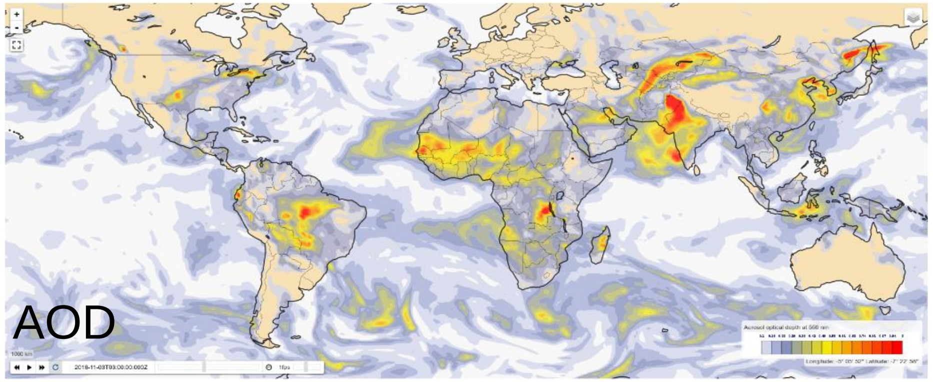
Transforming satellite observations into user-driven services.

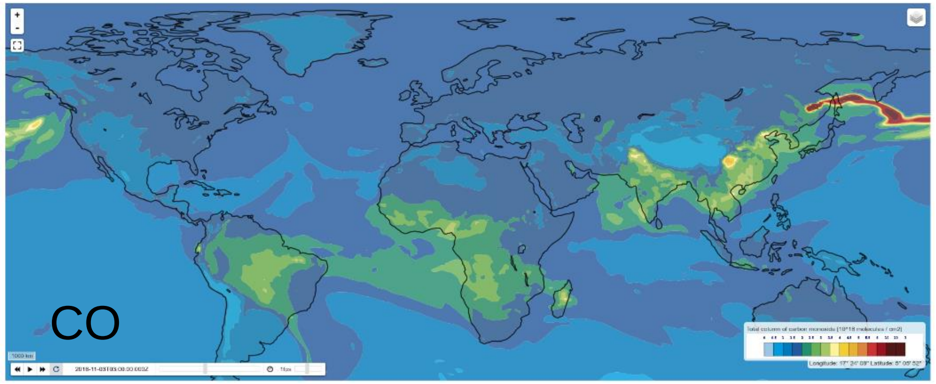


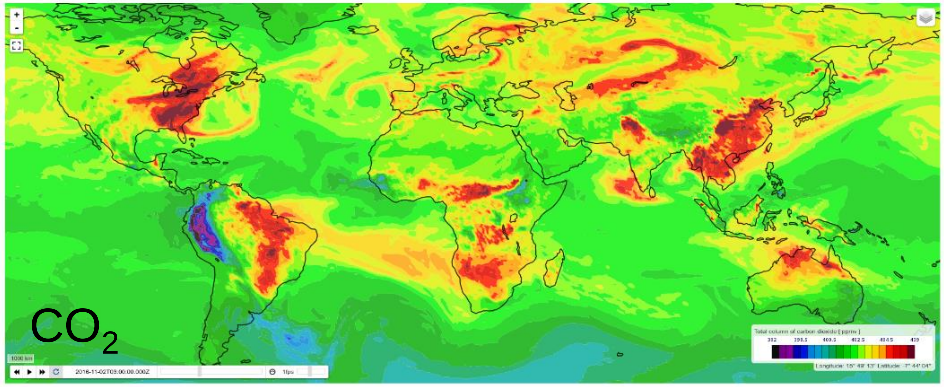


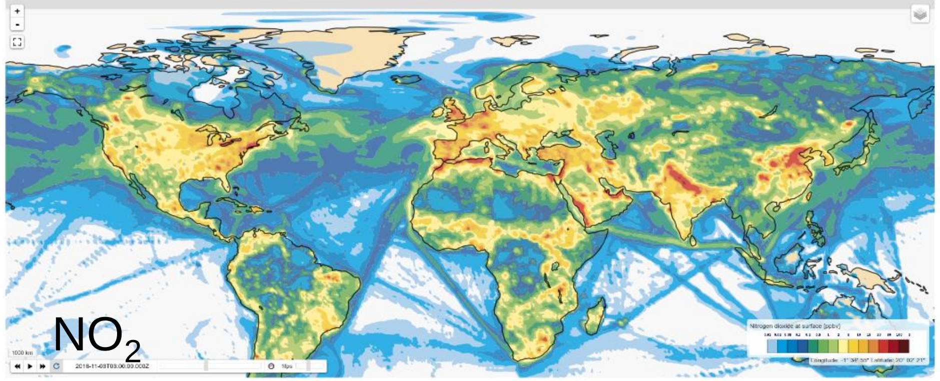
ECMWF EUROPEAN CENTRE FOR MEDIUM-RANGE WEATHER FORECASTS

Copernicus Global System









40km horizontal resolution at 60 model levels; two 5-day forecasts at 00z and 12z UTC each day

- **Aerosols (AOD and concentration): 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)

Data Assimilation Methodology for Atmospheric Composition

Data Assimilation Methodology

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

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

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

Atmospheric Composition models

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

Chemical module

GHG module

Aerosol module

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

Chemical module

GHG module

Aerosol module

Chemical Module

IFS

TM5 (CB05)
54 species, 126 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 CO2 by plants and release of CO2 by soil

CH4 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

12 aerosol-related prognostic variables:
3 bins sea-salt, 3 bins dust, Black carbon, Organic matter, Sulphate

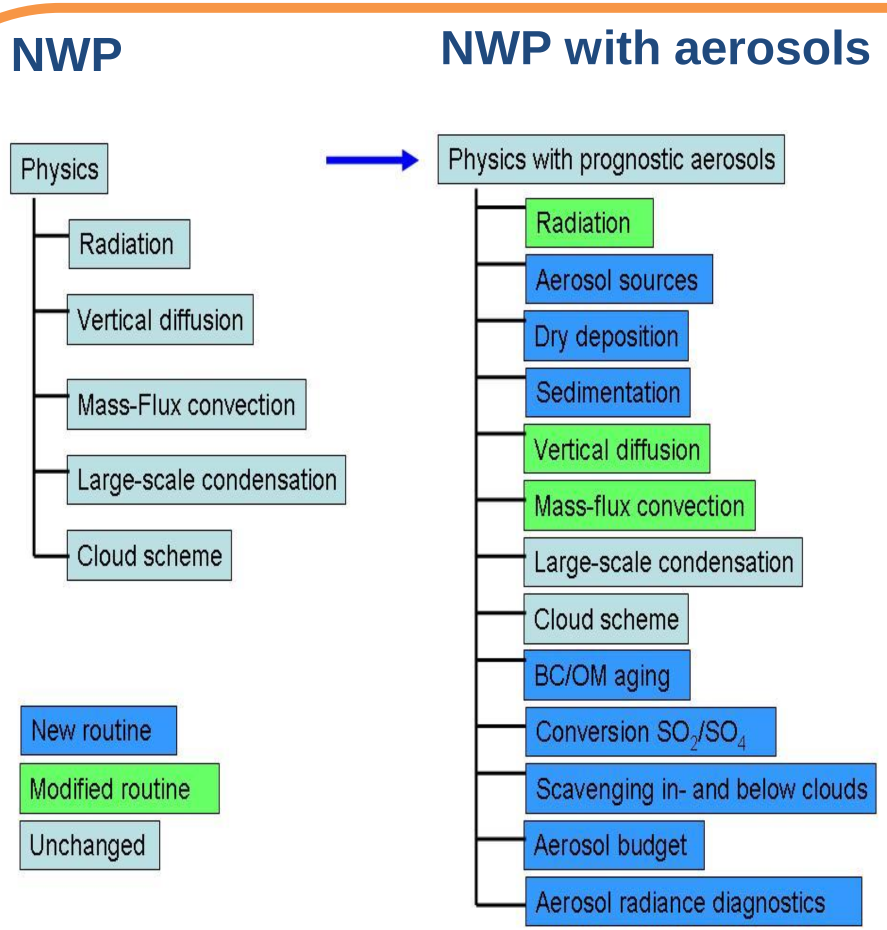
Emissions, dry and wet deposition, sedimentation

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

Data Assimilation Methodology

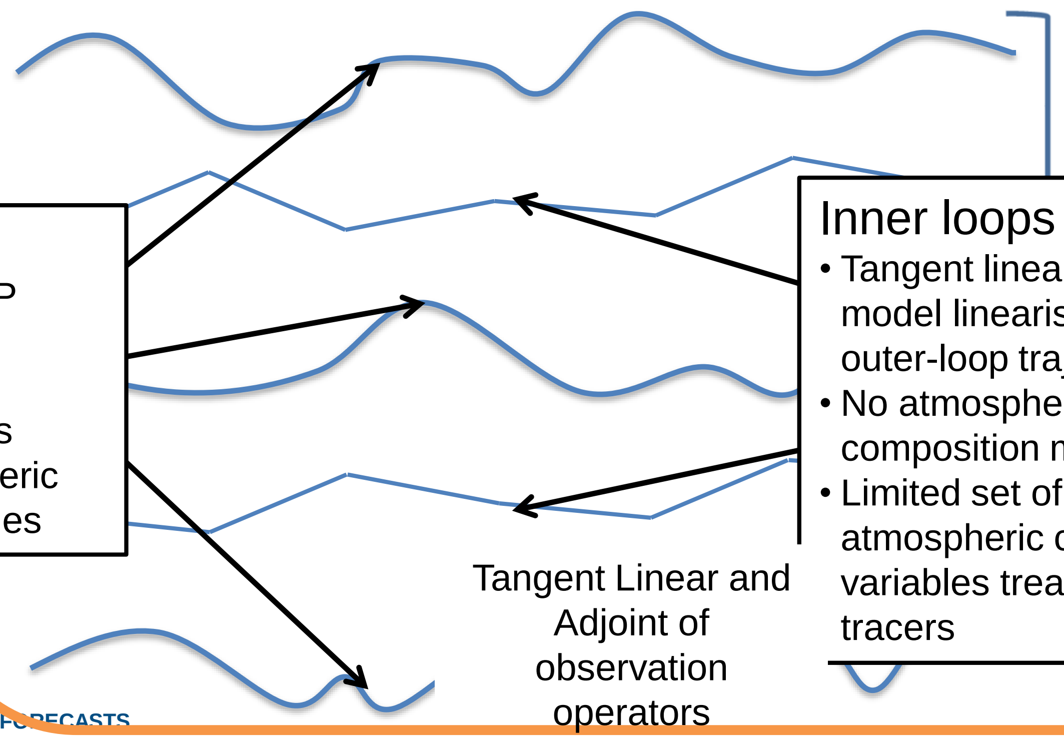
Data assimilation for atmospheric composition is in principle no different from NWP data assimilation

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

IFS

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

Incremental 4DVar



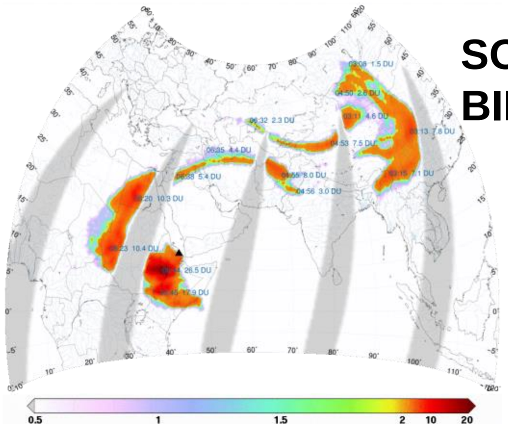
Outer loops
- Full non-linear NWP model
- Full atmospheric composition models
- Full set of atmospheric composition variables

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

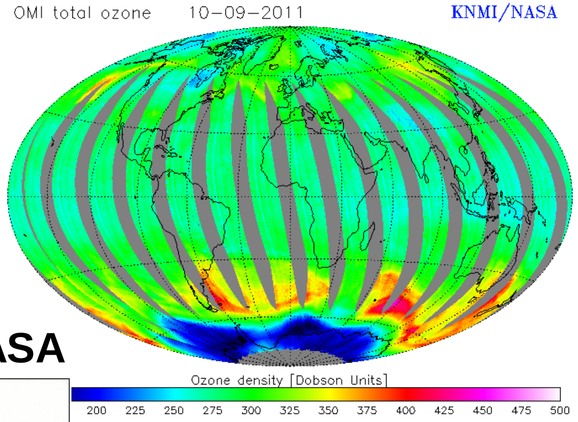
Observations of Atmospheric Composition

Satellite Observations

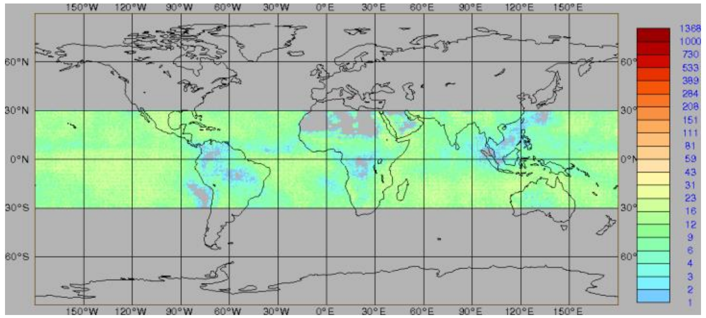
SO_2, GOME-2, SACS, BIRA/DLR/EUMETSAT



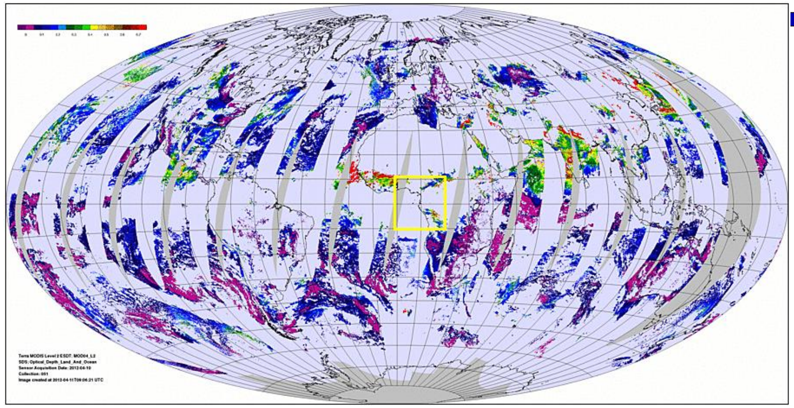
O_3, OMI, KNMI/NASA



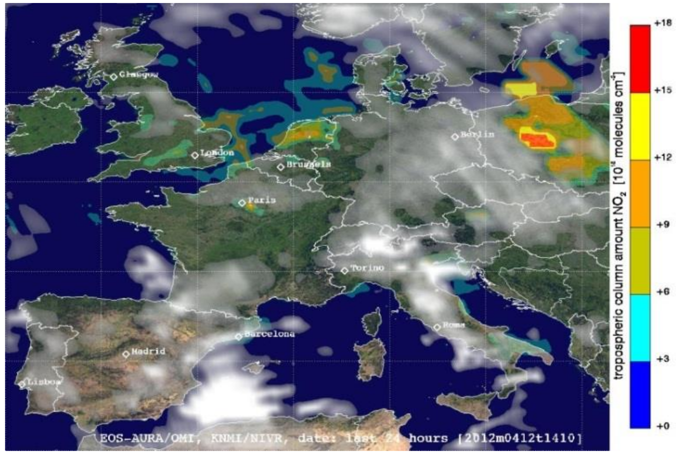
CH_4, IASI, LMD



Aerosol Optical Depth, MODIS, NASA

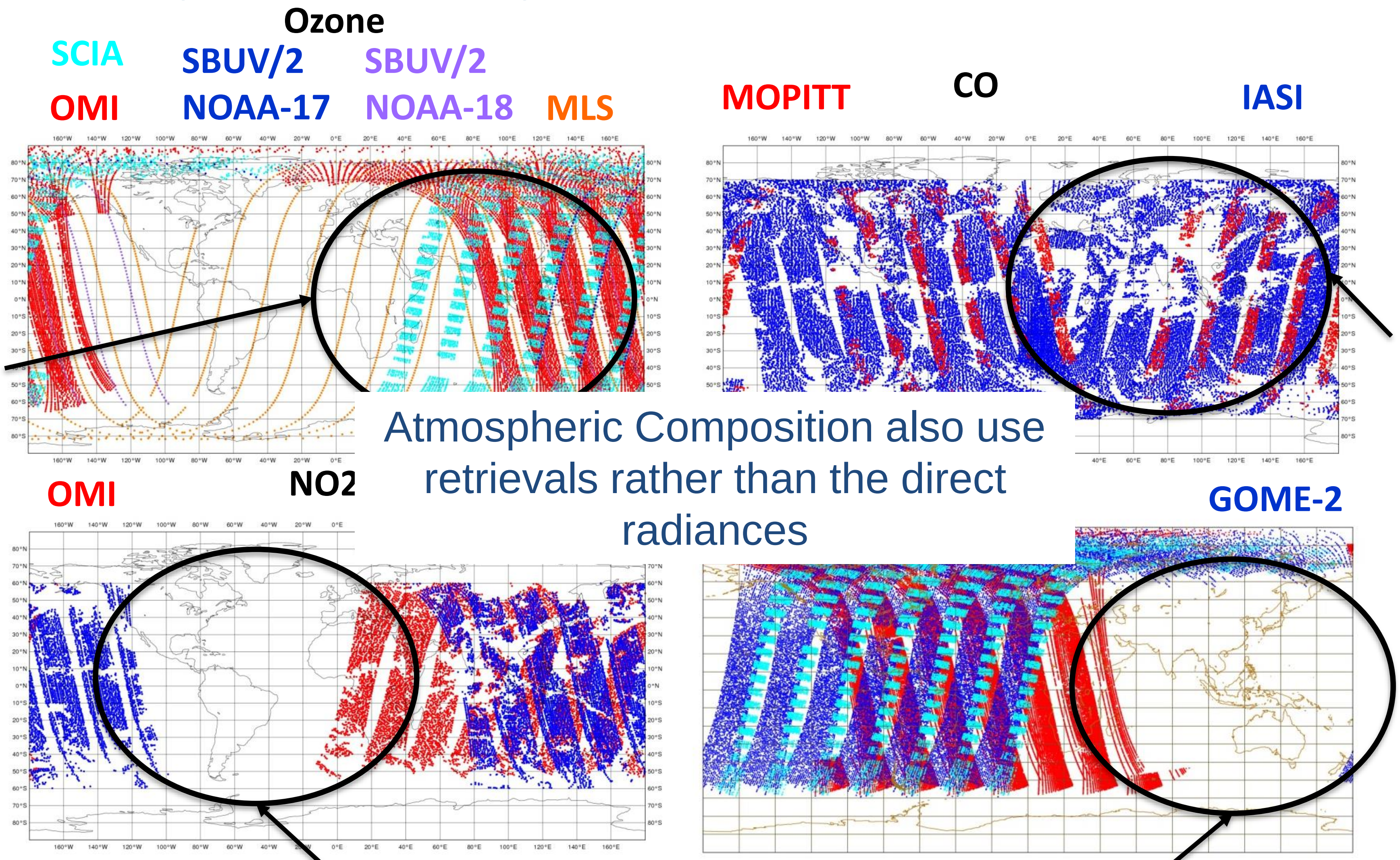


NO_2, OMI, KNMI/NASA



Atmospheric composition observations traditionally come from UV/VIS measurements. This limits the coverage to day-time, cloud-free only. Infrared/microwave are now adding more and more to this spectrum of observations (MOPITT, AIRS, IASI, MLS, MIPAS …)

NRT data coverage for reactive gases



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

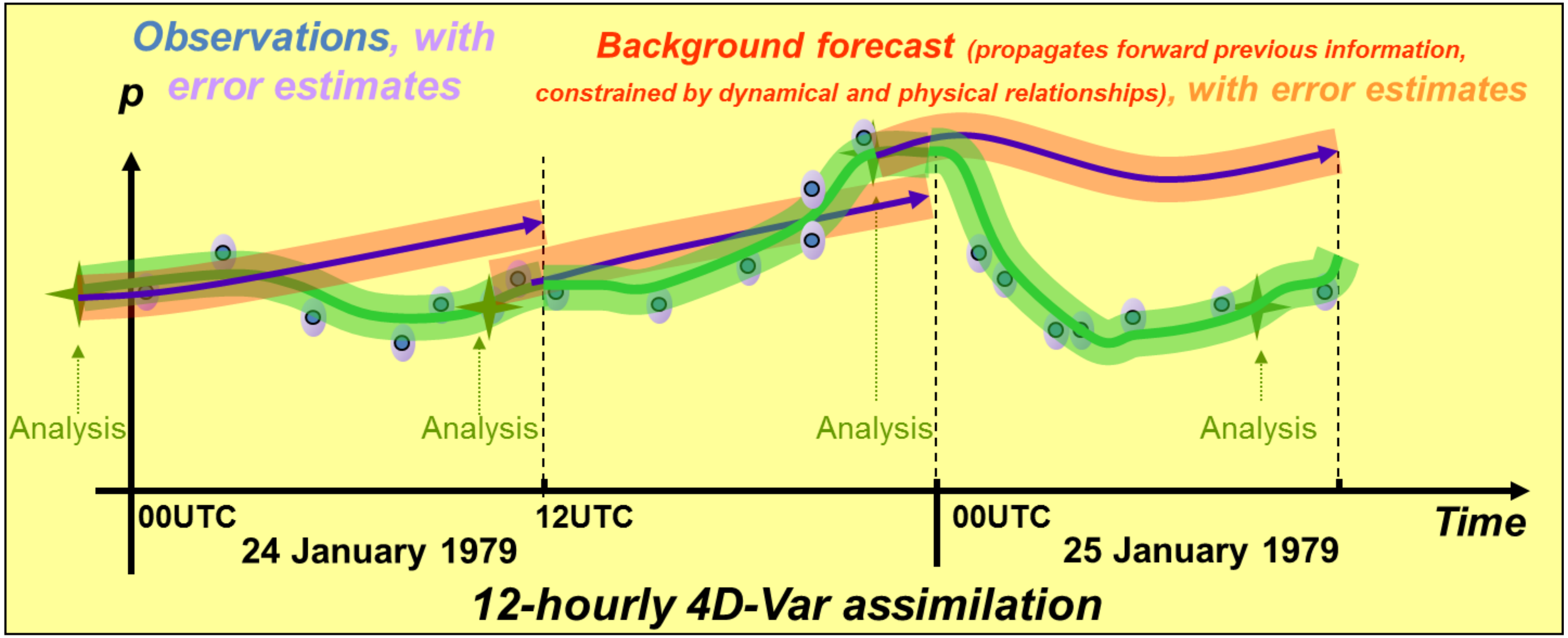
Often limited to cloud free conditions

Atmospheric Composition also use retrievals rather than the direct radiances

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

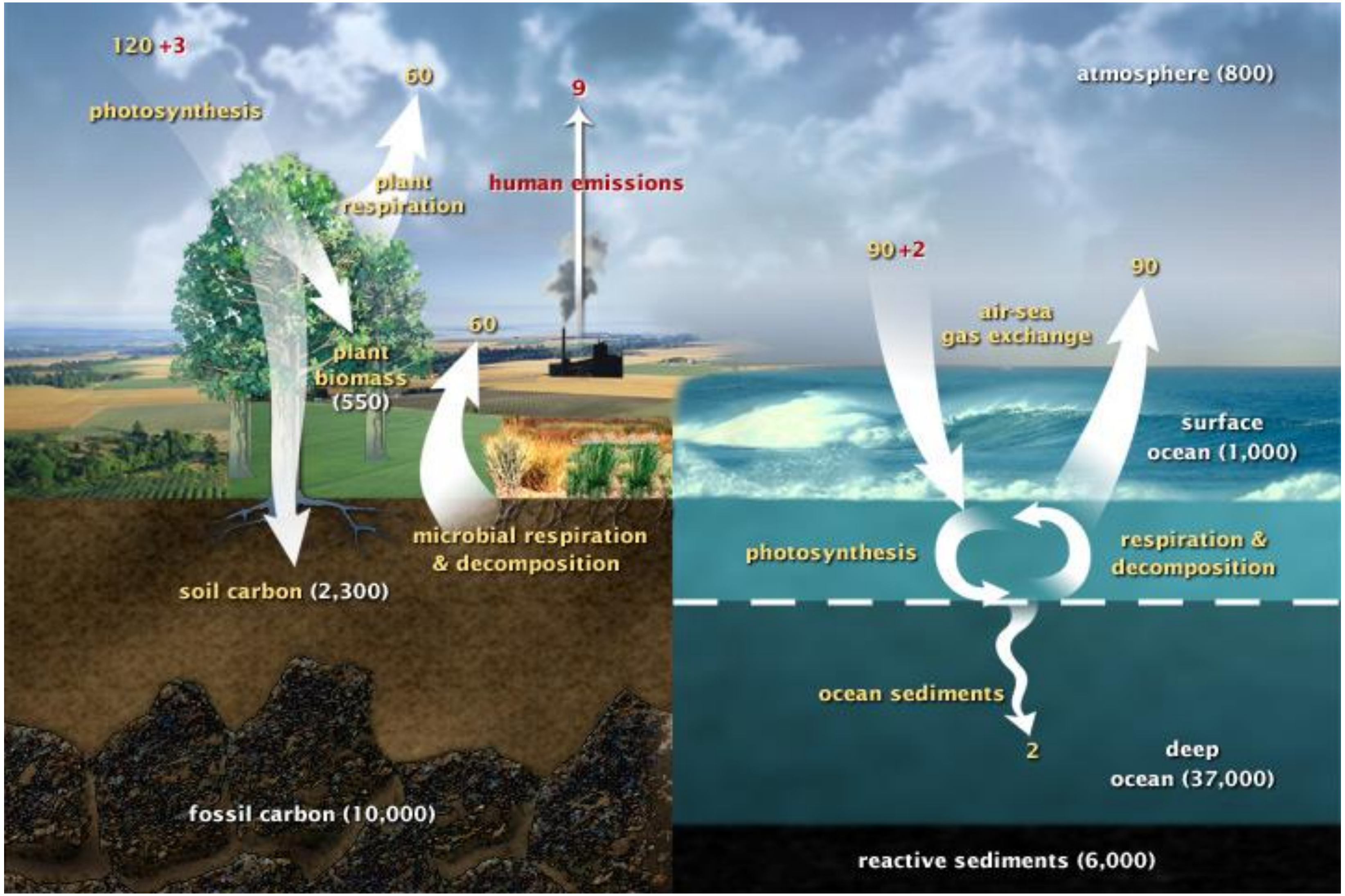
Challenges for Atmospheric Composition Data Assimilation

1. Initial vs Boundary Problem



- 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 model parameters (e.g. emissions, deposition, reaction rates, …)

Surface fluxes



An example of all the surface fluxes that need to be accounted for with CO_2

Emission Processes

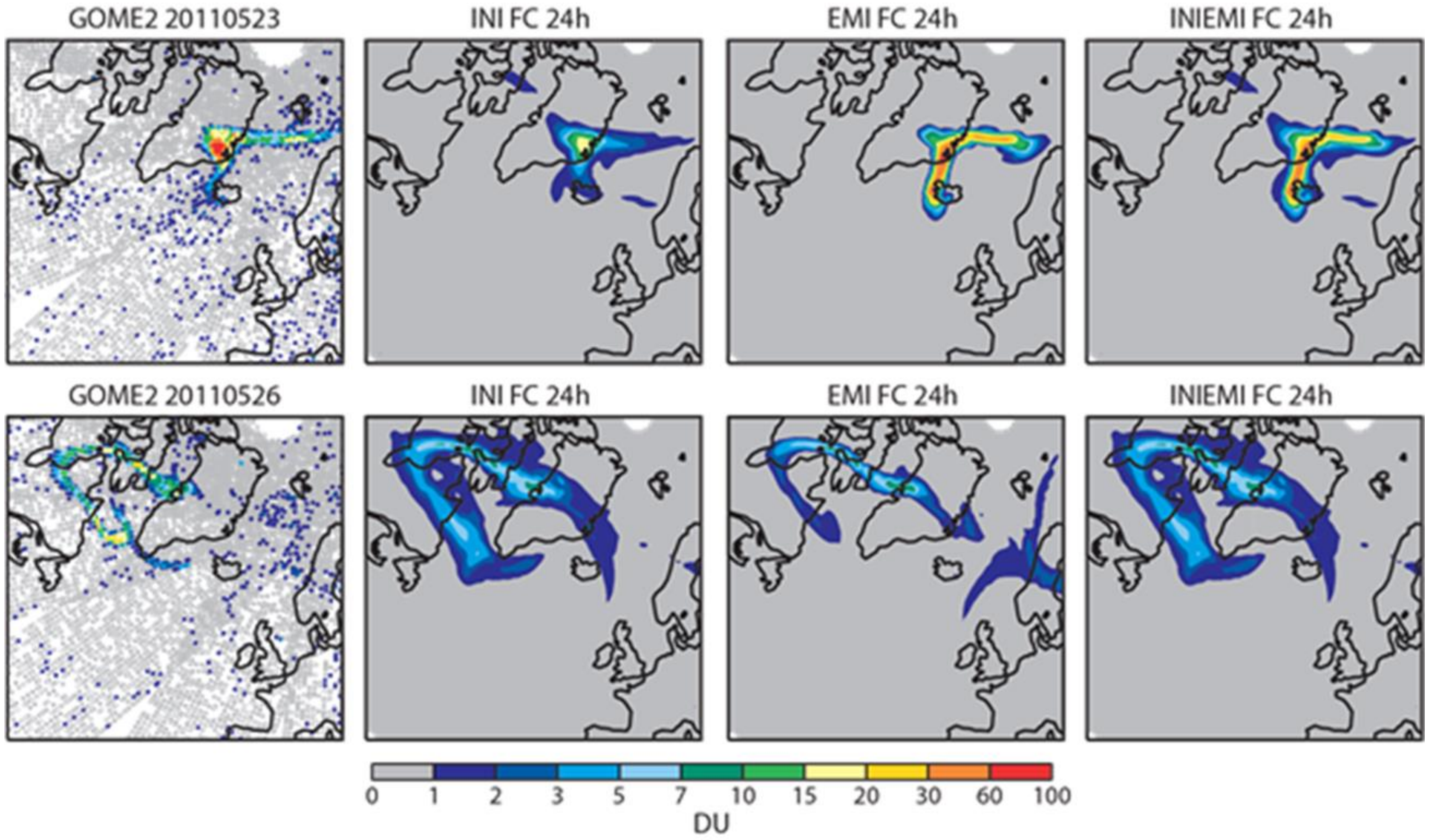
- Combustion related (CO, NO_x, SO_2, VOC, CO_2):
  - Fossil fuel combustion
  - Biofuel combustion
  - Vegetation fires (man-made and wild fires)

- Fluxes from biogeochemical processes (VOC, CH4, CO_2, Pollen):
  - Biogenic emissions (plants, soils, oceans)
  - Agricultural emissions (incl. fertilisation)

- Fluxes from wind blown dust and sea salt (from spray)

- Volcanic emissions (ash, SO_2, HBr …)

Example: volcanic eruptions



Plume close to source

Plume away from source

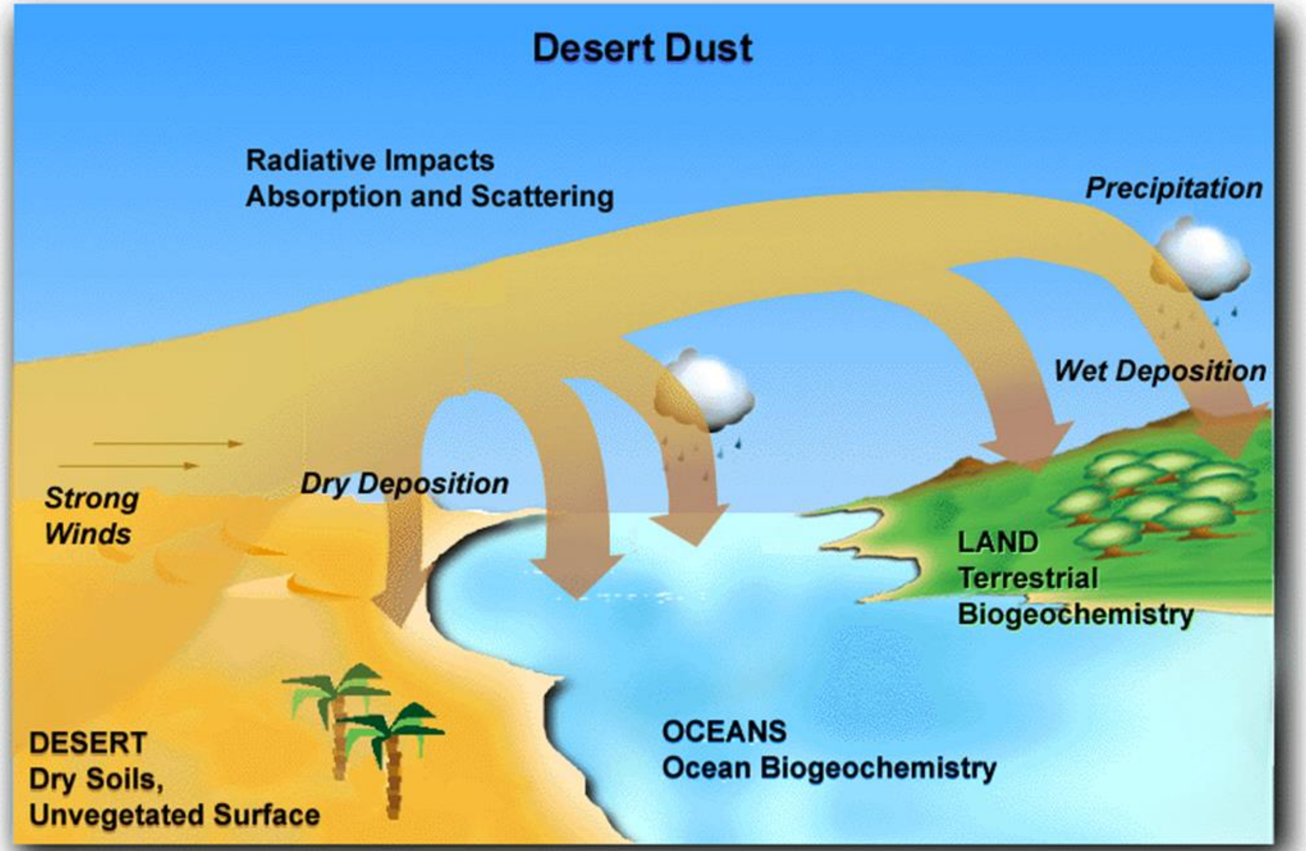
Both initial conditions and emissions are important to get it right

Emission Estimates

- Emissions are one of the major uncertainties in 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 (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 – in particular for long lived gases such as CO2 (e.g. Chevallier et al. 2014) and Methane (Bergamaschi et al. 2009)

How to improve?

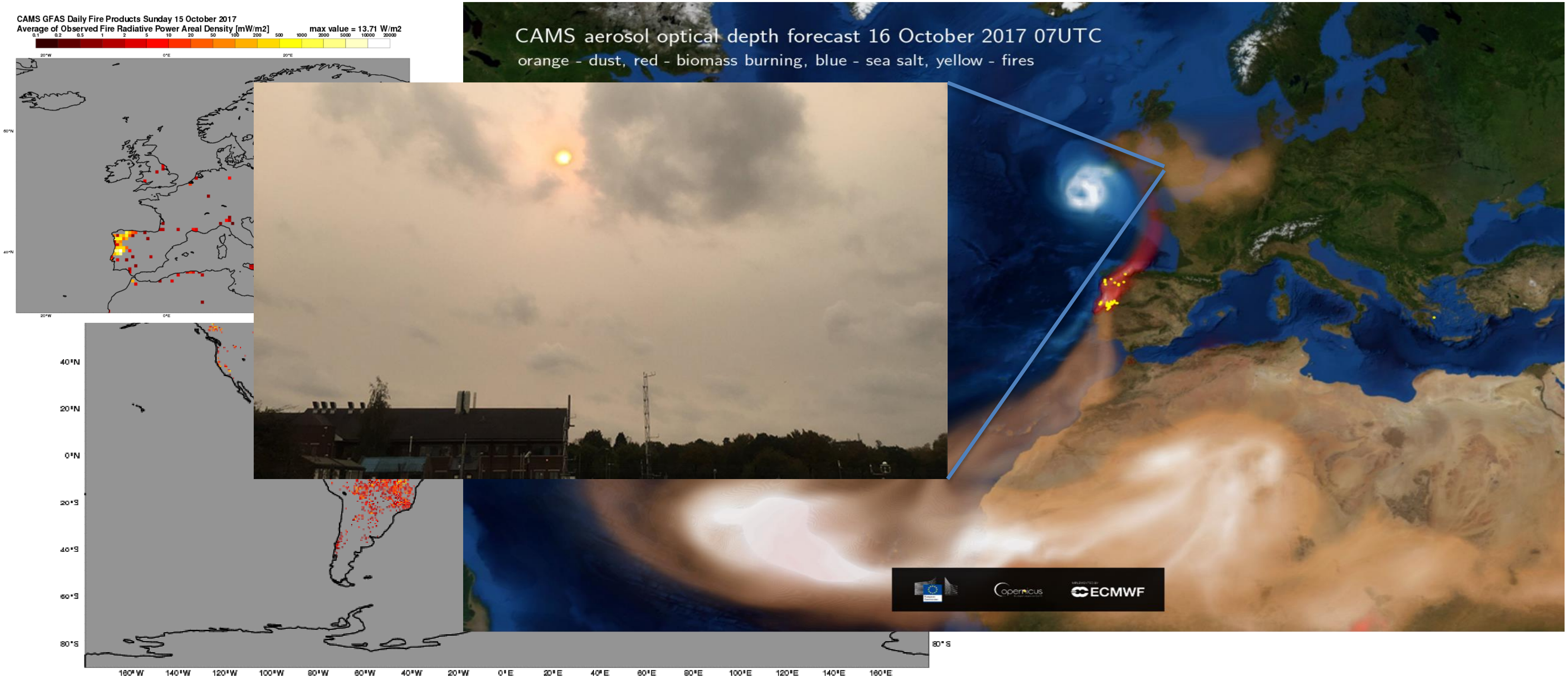
Better modelling of fluxes and emissions



Modelling of sea salt and desert dust fluxes.

How to improve?

Use near-real-time off-line estimates of emissions



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

Doubles the computation time

+

Future 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 correction factor since we already know a lot about emissions?

Include as model error?

2. Mismatch between modelled and observed variables

$$J(x) = (x$$

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

Control variables

NWP

vorticity
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temperature
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Atmospheric Composition

ozone
carbon monoxide
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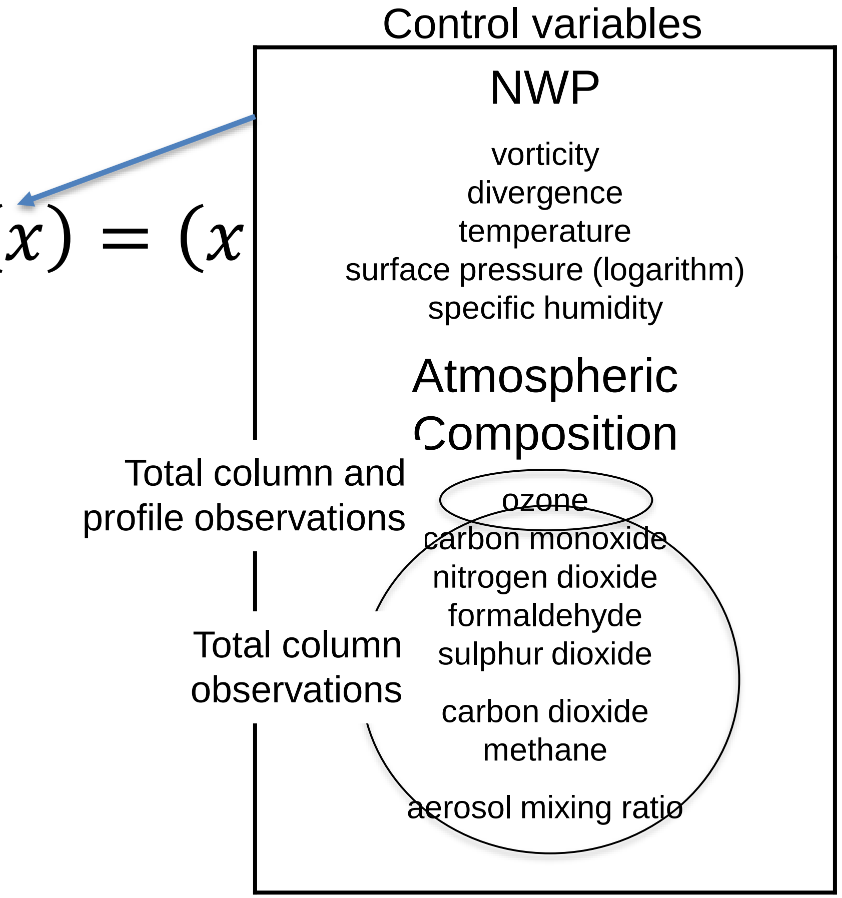
aerosol mixing ratio

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.

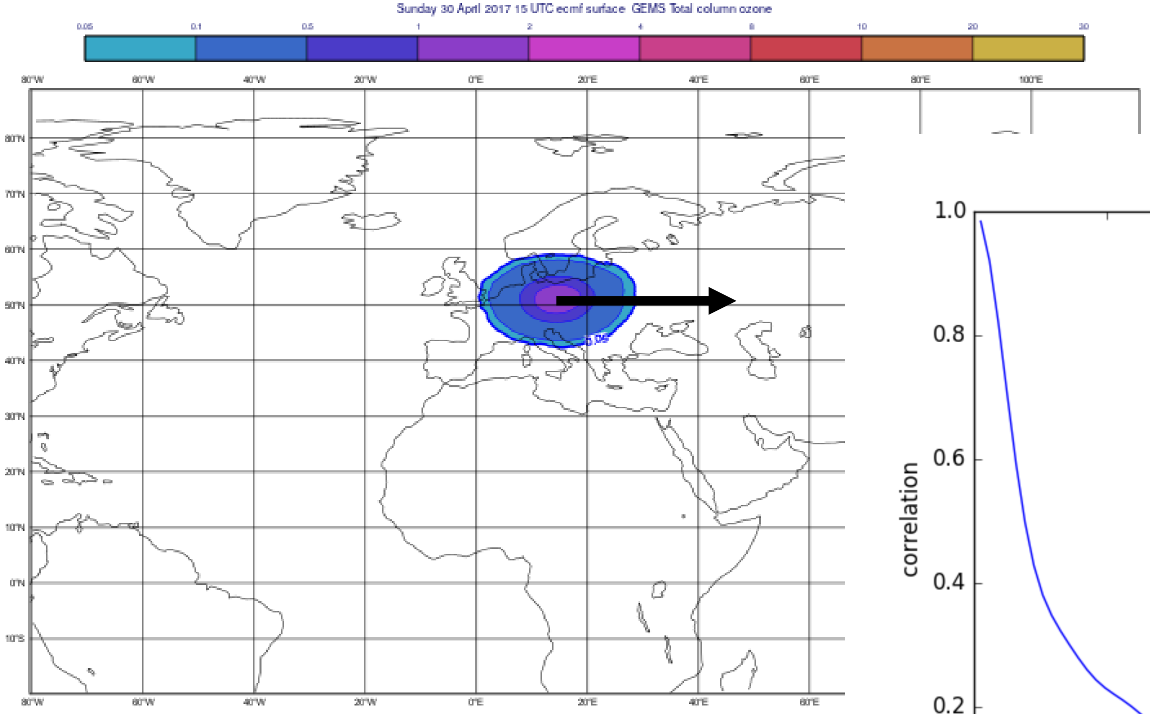
2. Mismatch between modelled and observed variables

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

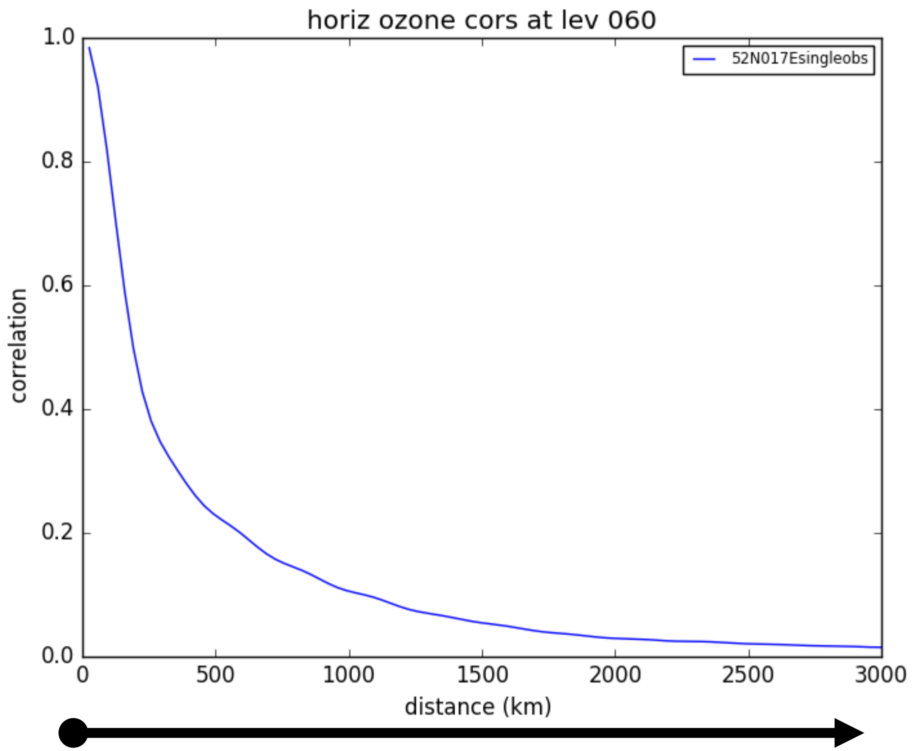


Even for those species that are observed, it is often only total column data that is available.

Increment from a single total column ozone observation

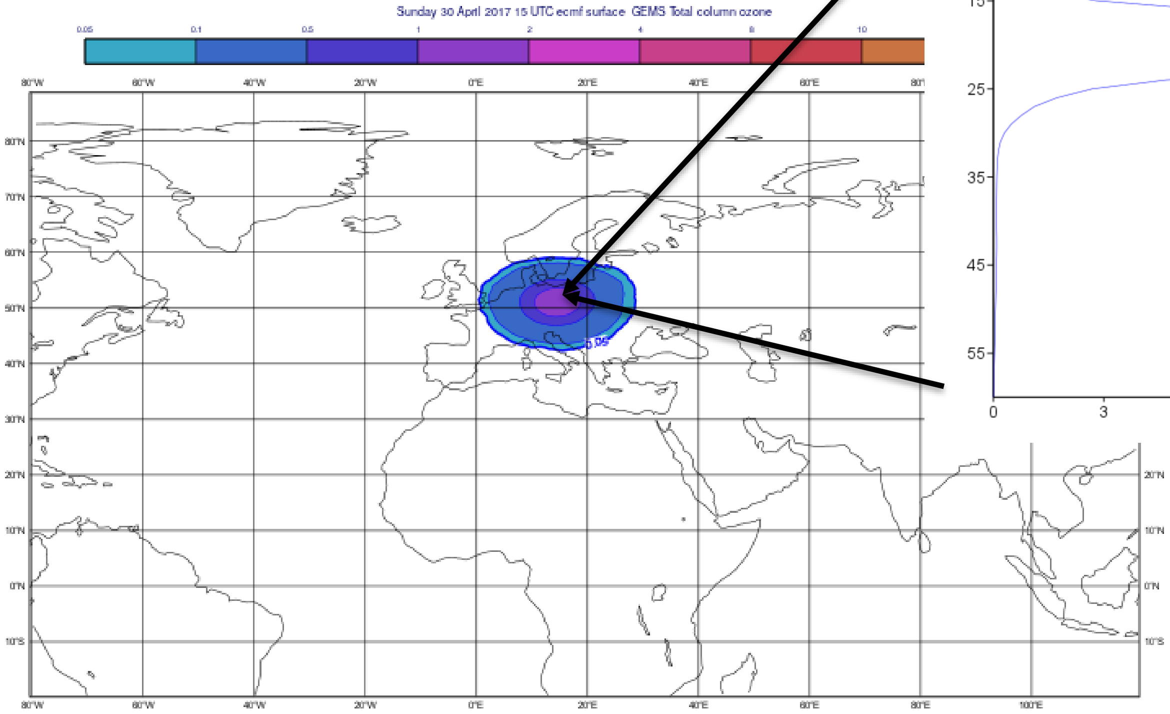


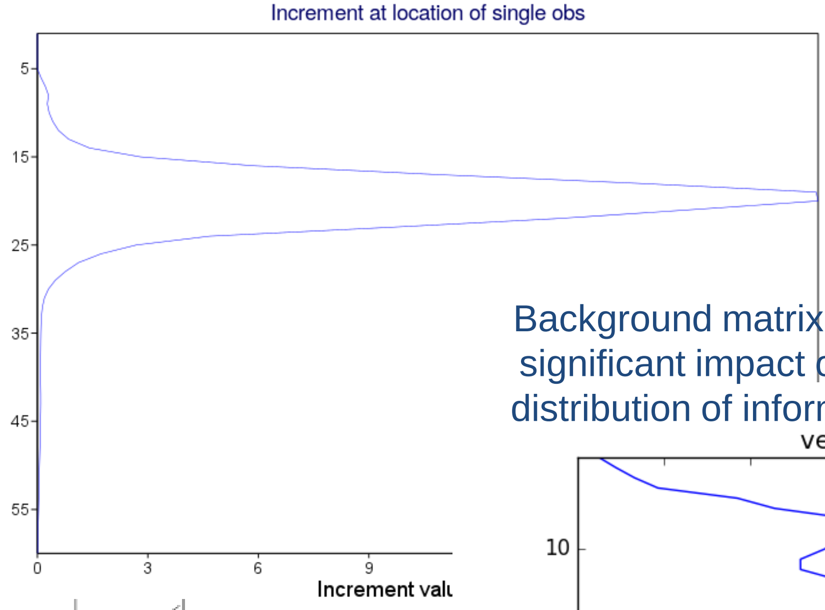
Increment created by a single ozone observation of 375 DU, 10 DU higher than background



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

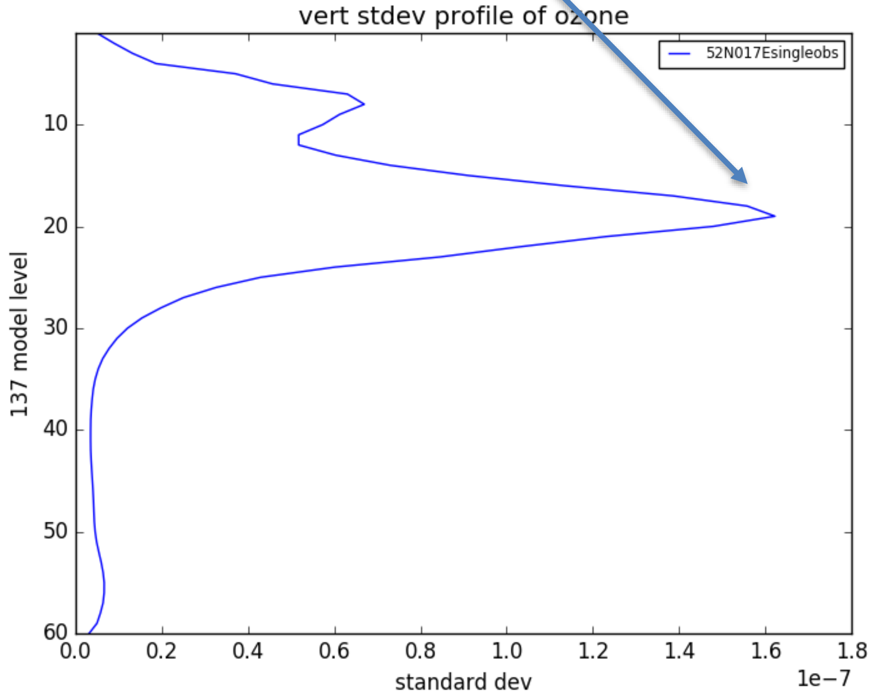
Increment from a single total column ozone observation





Vertical profile of the increment at the observation location

Background matrix has a significant impact on the distribution of information

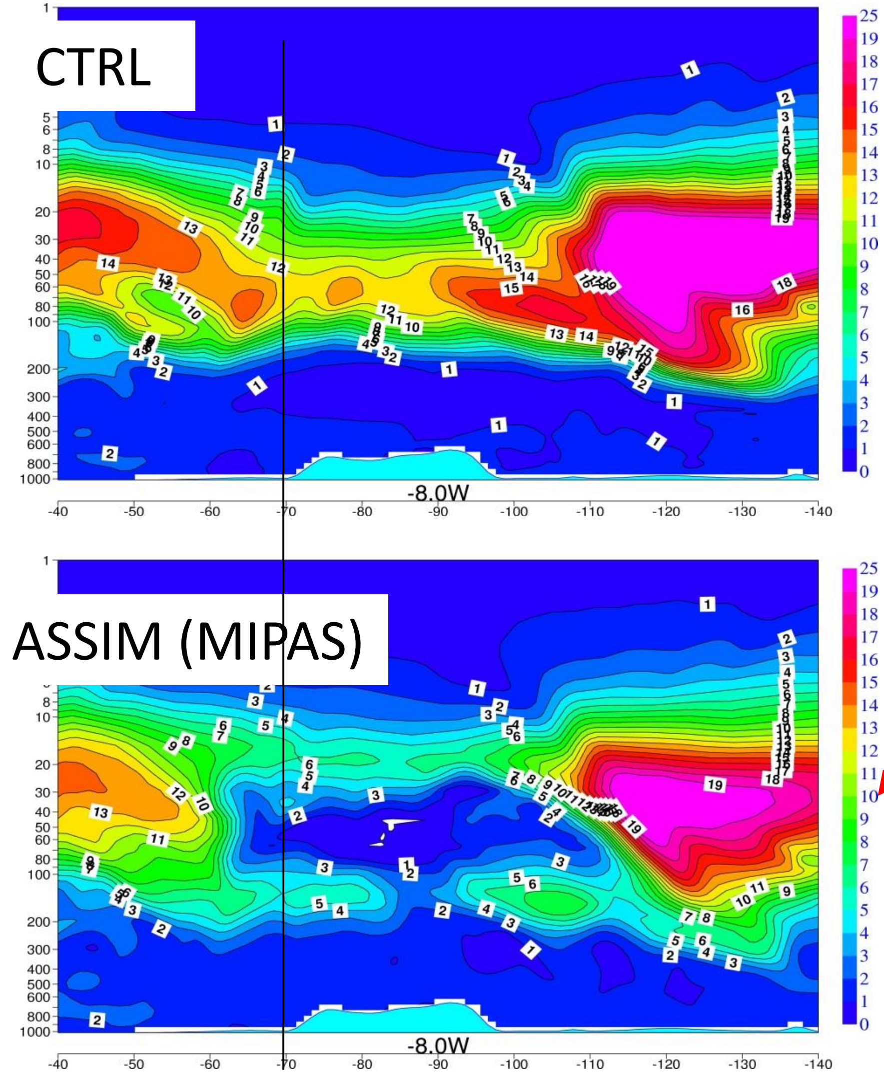


Increment created by a single ozone observation of 375 DU, 10 DU higher than background

Standard deviation from the background matrix at the observation location

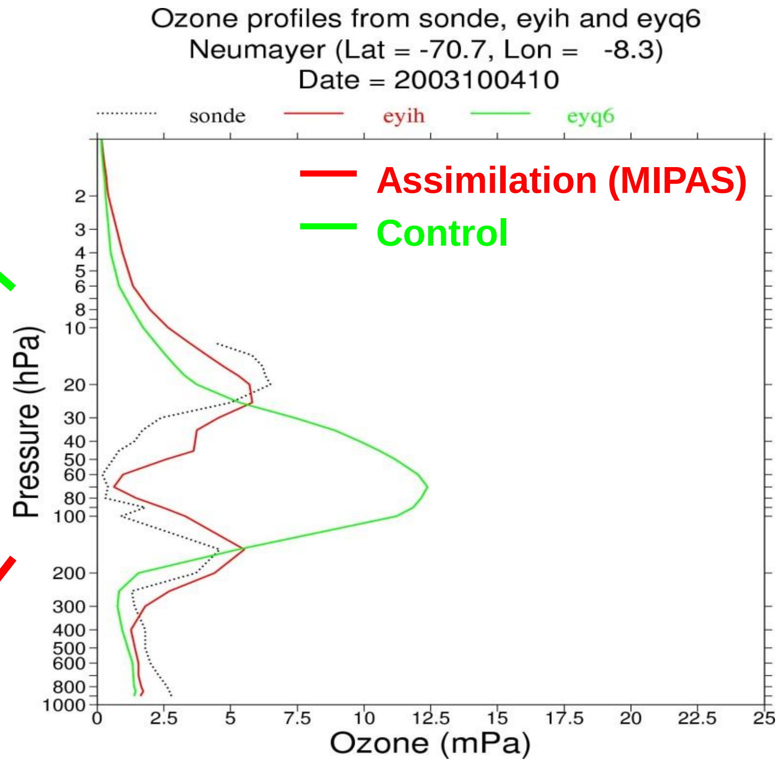
Formulation of the B-matrix is very important for AC

Benefit of profile information – B matrix is not enough!



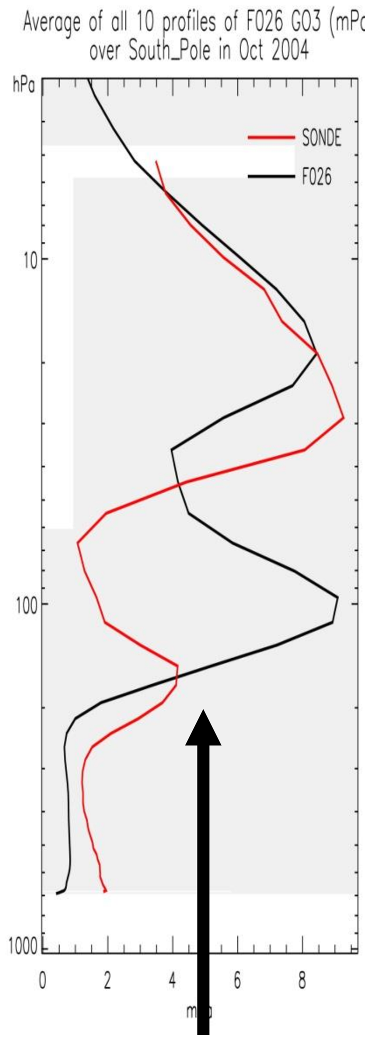
70S

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



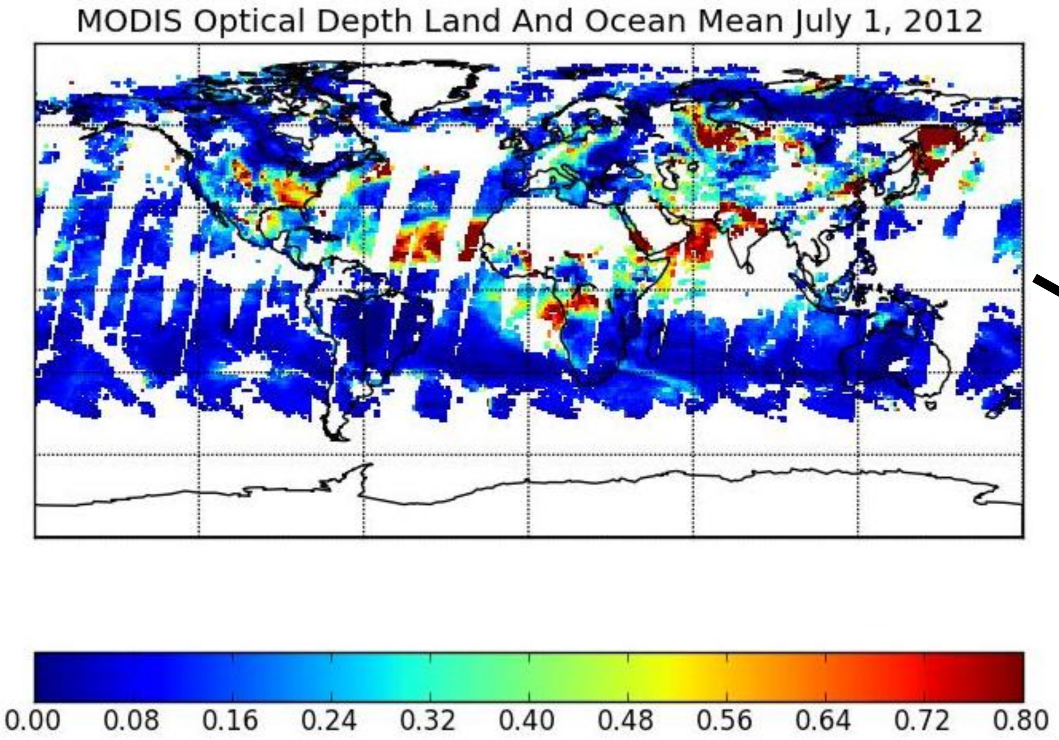
Assimilation **with profile data**

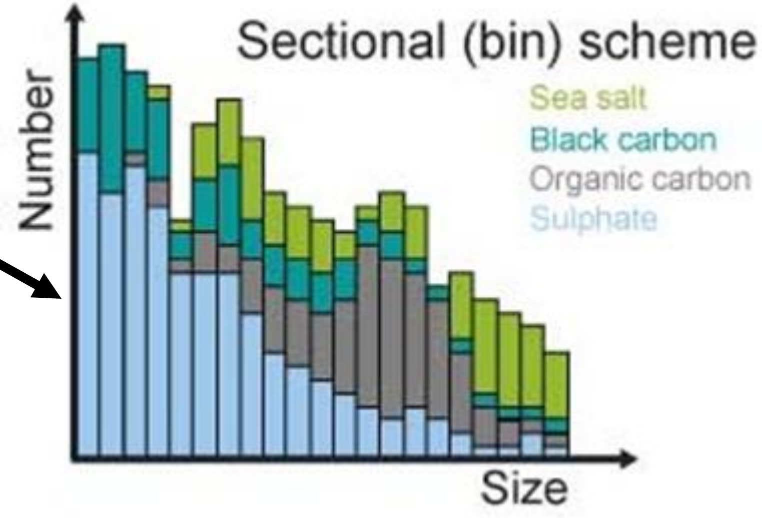
Oct 2004



Assimilation **with total column data**

Added difficulty with AOD observations





AOD observations used in the assimilation → Bin scheme model used with 12 bins

How to transfer the information from the total aerosol to the 12 difference bins? B-matrix is not relevant in this case…

Added difficulty with AOD observations

Nonlinear run:

- All bins/species are initialized from a previous forecast; the total aerosol mixing ratio is initialized from sum of all bins/species.
- All aerosol variables go through advection, vertical diffusion and convection.
- Individual bins/species mixing ratio are used to compute optical depth according to the bin/species-specific optical properties.

Tangent linear/adjoint runs:

1. Perturbations of optical depth are started from zero perturbations on individual bin/species mixing ratios on the first call of the tangent linear.
2. These perturbations are then passed to the adjoint routine to compute the gradient wrt individual bin/species mixing ratios. The gradient in the total aerosol mixing is then obtained from

$$r_t^* = \sum_i f_i r_i^*$$

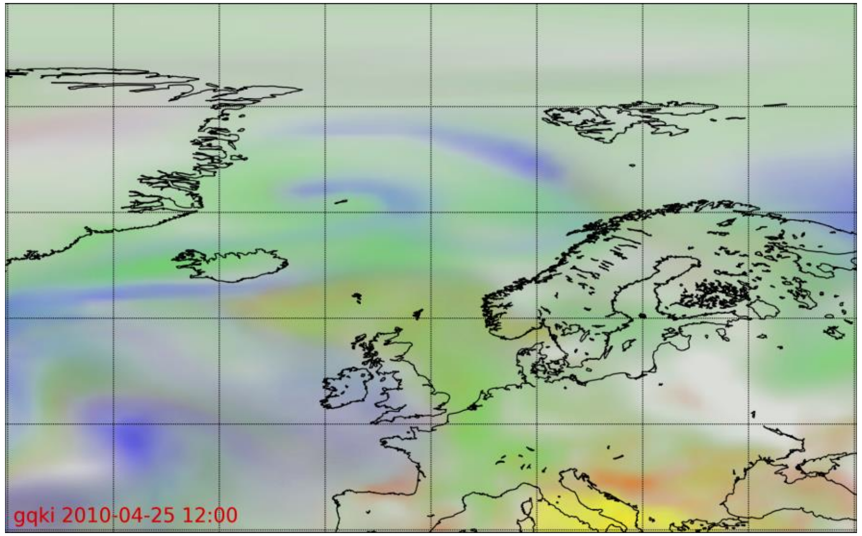
   where f_i represents the fractional contribution of each bin/species to the total mixing ratio.

3. The gradient wrt total aerosol mixing ratio is then used in the minimization and the resulting increment in r_t is used in the tangent linear run to compute updated perturbations on the individual bin/species mixing ratios as follows:

$$r_i' = f_i r_t'$$

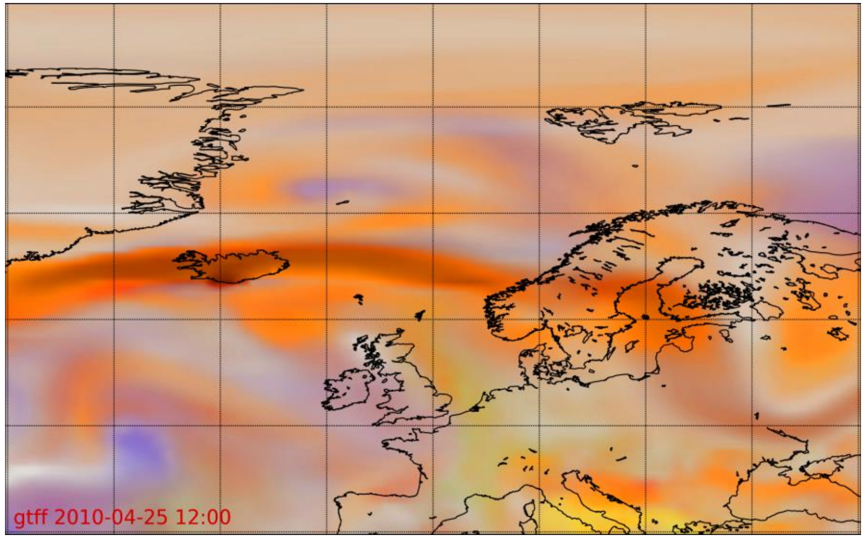
   This last step is not fully justifiable unless $r_t = \sum_i r_i$ at all times and at all locations.

Added difficulty with AOD observations



Assimilating Aerosol Optical Depth (AOD) observations without having all required aerosol species realistically in place, results in wrong species assignment in analysis (plume of organic matter aerosol above).

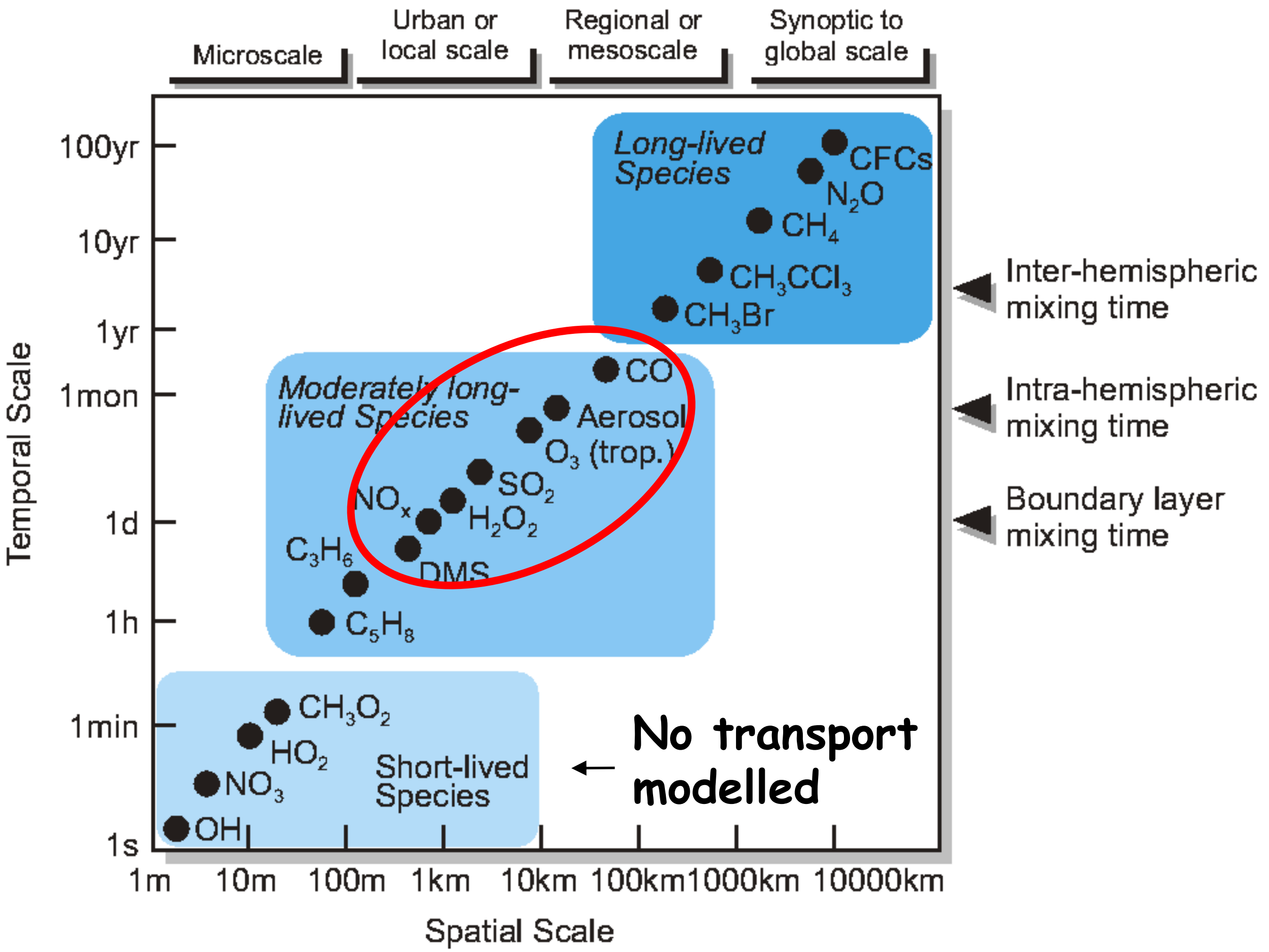
Improving the model with estimated emissions of volcanic ash and sulphates (below) allows much better use of observations.



Sea-salt
Dust
Organic matter
Background sulphate
Volcanic ash
Volcanic sulphate

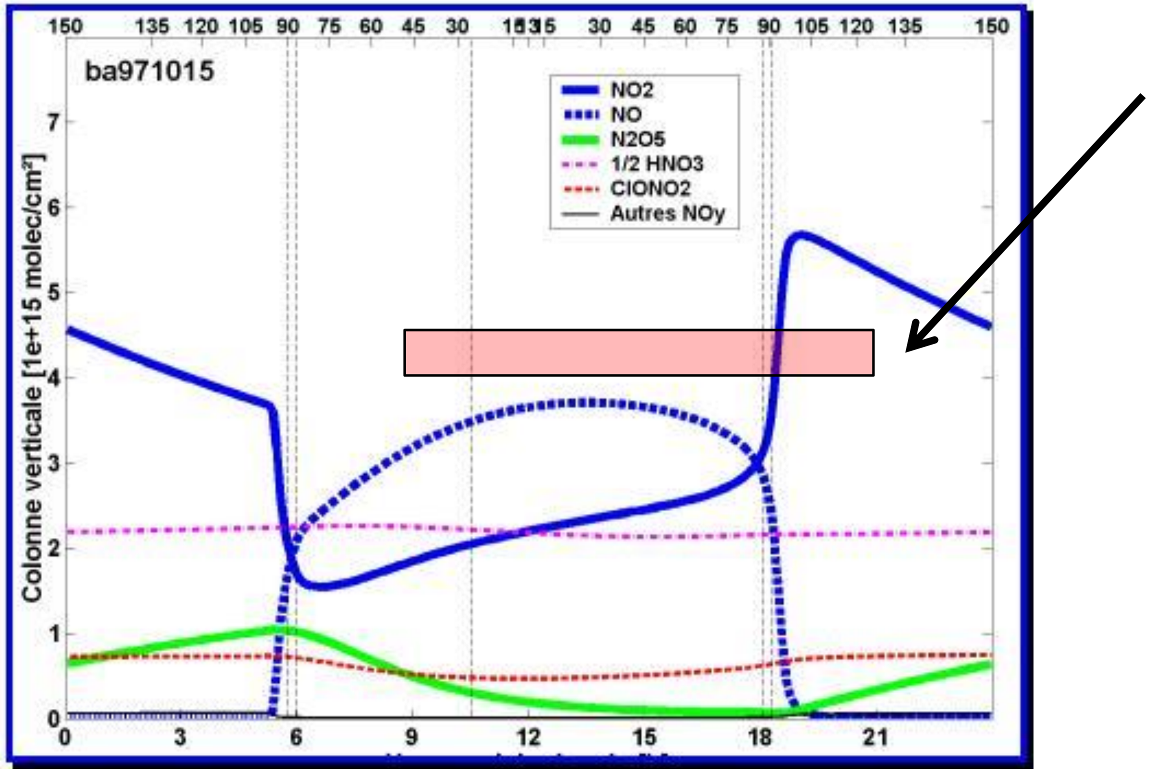
Volcanic eruptions Eyjafjallajökull

3. Lifetime of species



After Seinfeld and Pandis [1998]

NO_2 data assimilation



12-hour 4D-Var window

Rapid chemical conversion within the 12-hour 4D-Var window means we cannot link an NO2 observation at the end of the window correctly to the initial state without a full chemical adjoint.

$$NO_2 + \text{sunlight} \rightarrow NO + O$$

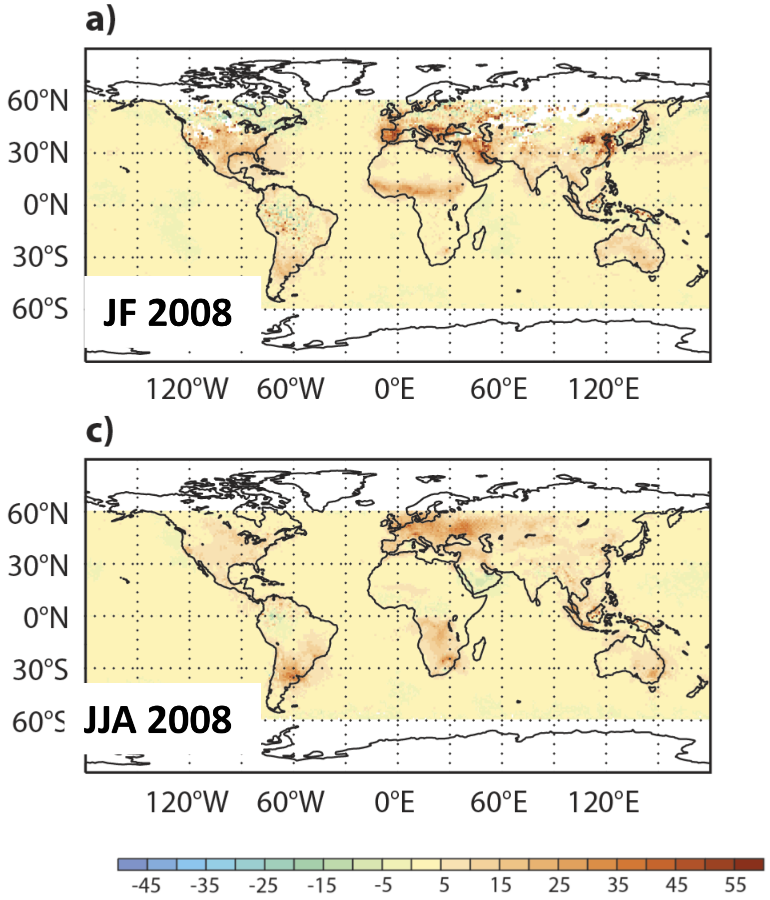
$$NO + CH_3O_2 \rightarrow NO_2 + CH_3O$$

Partial solution through simple approximation of main chemical reaction

$$\frac{[NO_2]}{NO_x} \approx \frac{k[O_{3eff}]}{JNO_2 + k[O_{3eff}]}$$

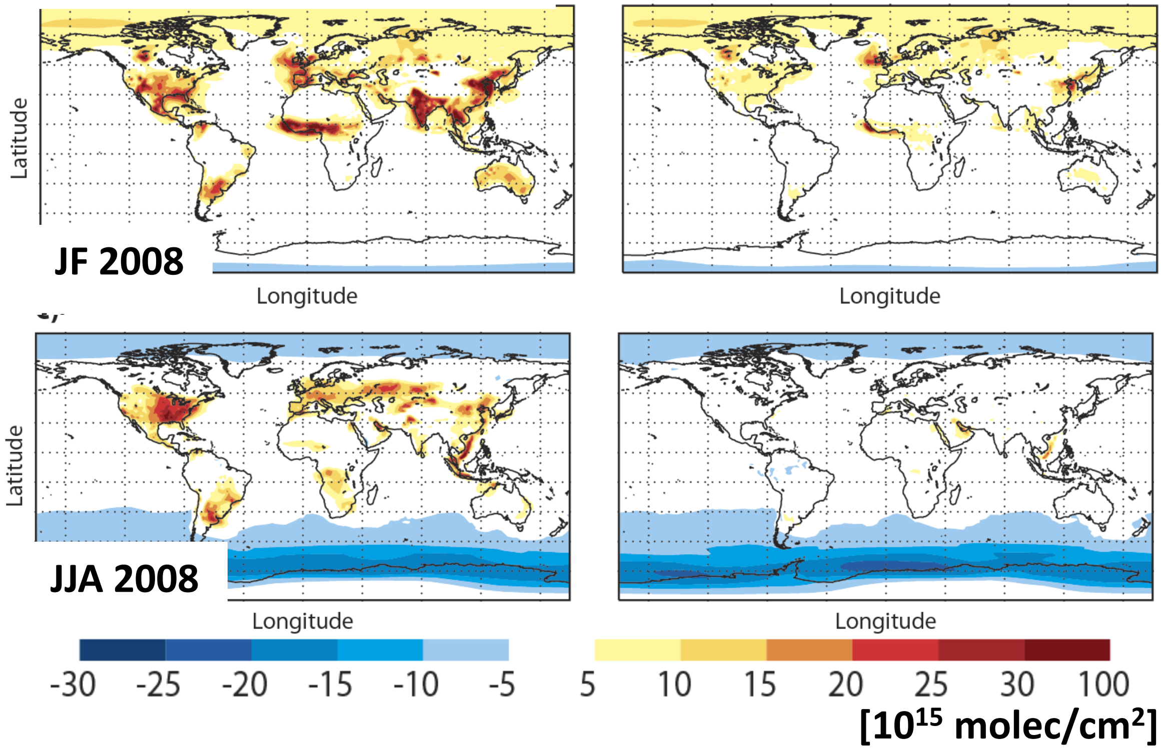
Short lived memory of NO2 assimilation

OMI NO2 analysis increment [%]



Differences between

Analysis and CTRL | **12h fc from ASSIM and CTRL**



- Large positive increments from OMI NO2 assim
- Large differences between analyses of ASSIM and CTRL
- Impact is lost during subsequent 12h forecast
- It might be more beneficial to adjust emissions (instead of IC)

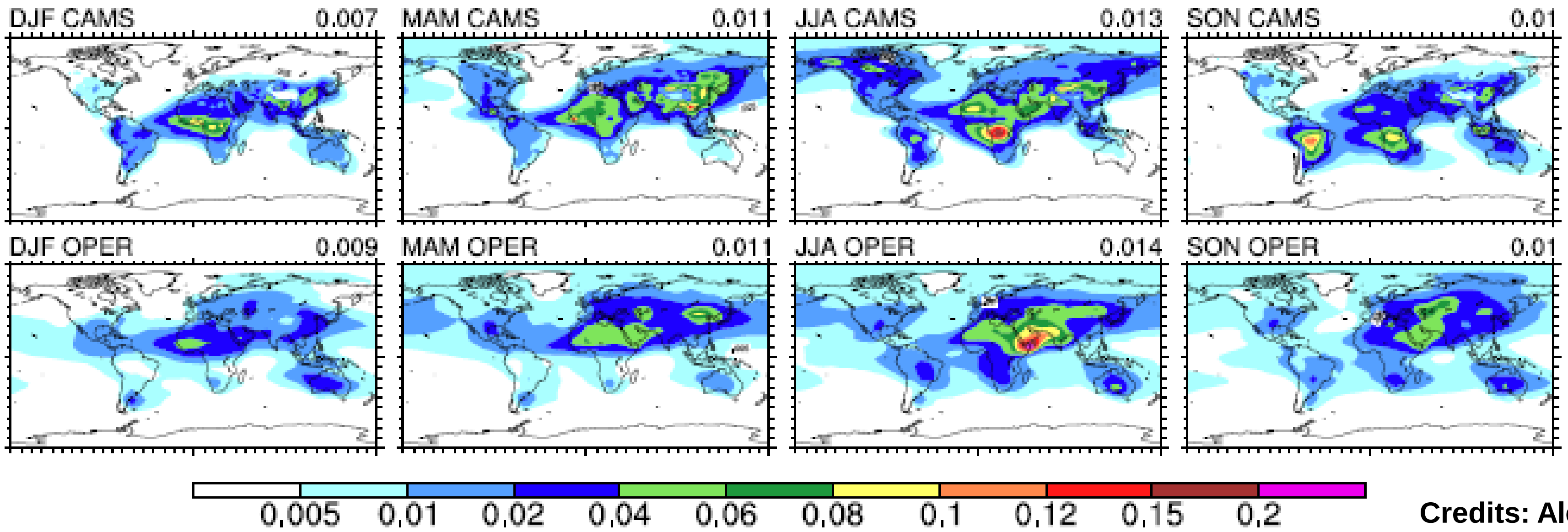
Potential Benefit for NWP

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
- Multivariate JB: Correlations between tracers and dynamical variables, e.g. O3 and vorticity; correlations between chemical species: univariate

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

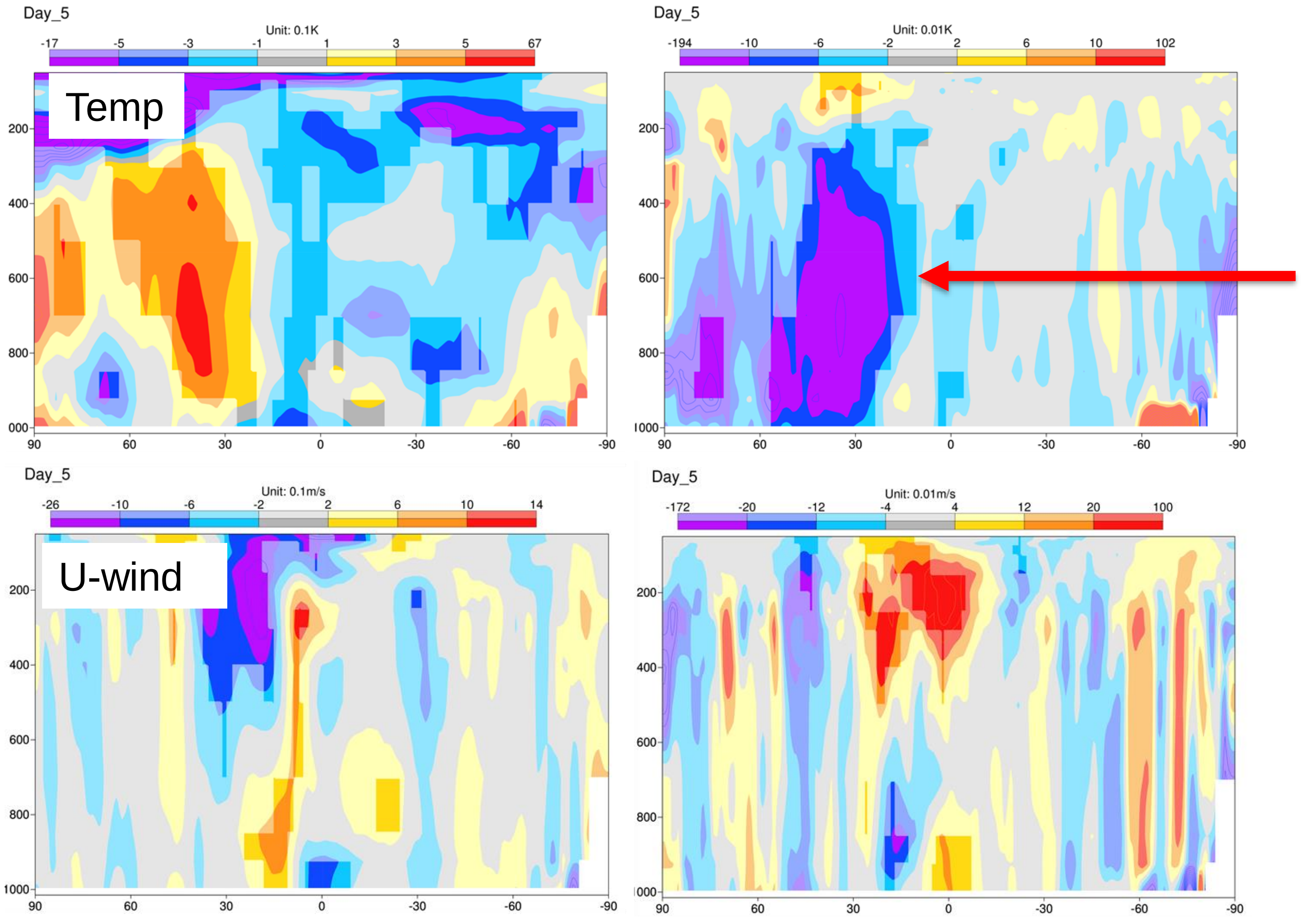
Climatological AOD 550nm distribution CAMS vs Tegen et al 1997



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



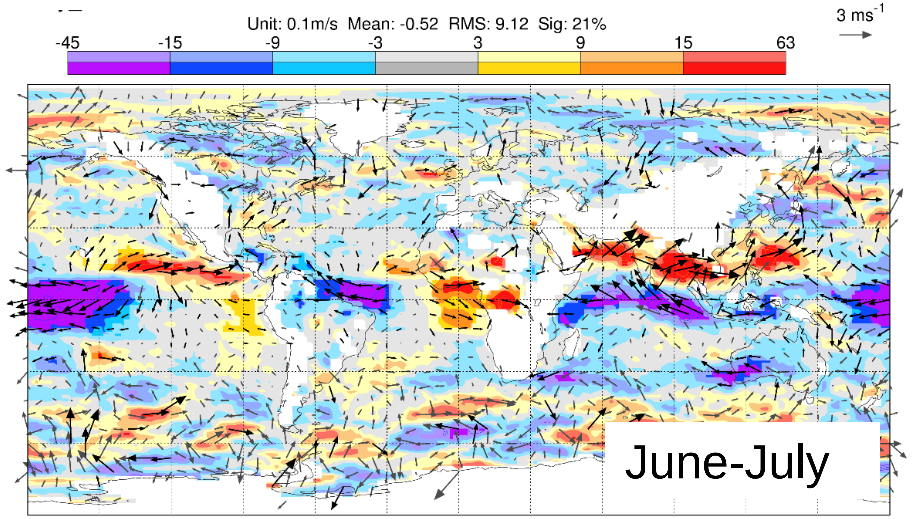
June-July
Model FC error d+5

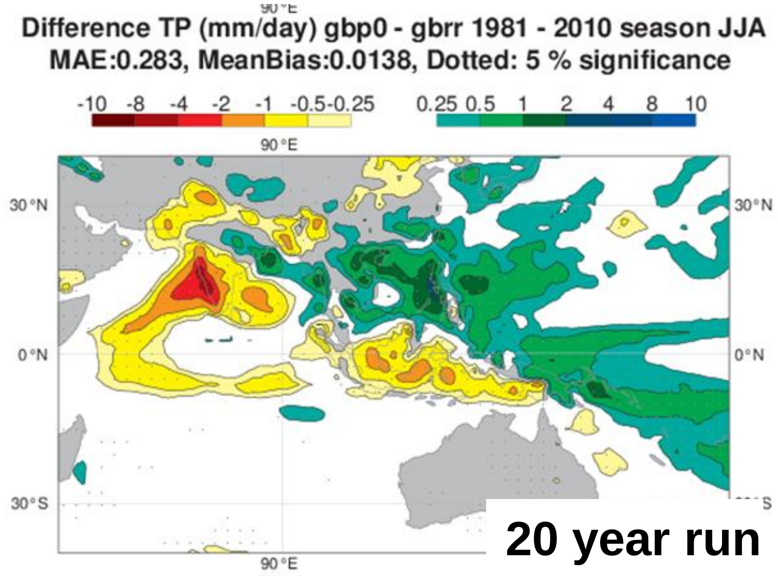
June-July
Change in FC error d+5

- 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

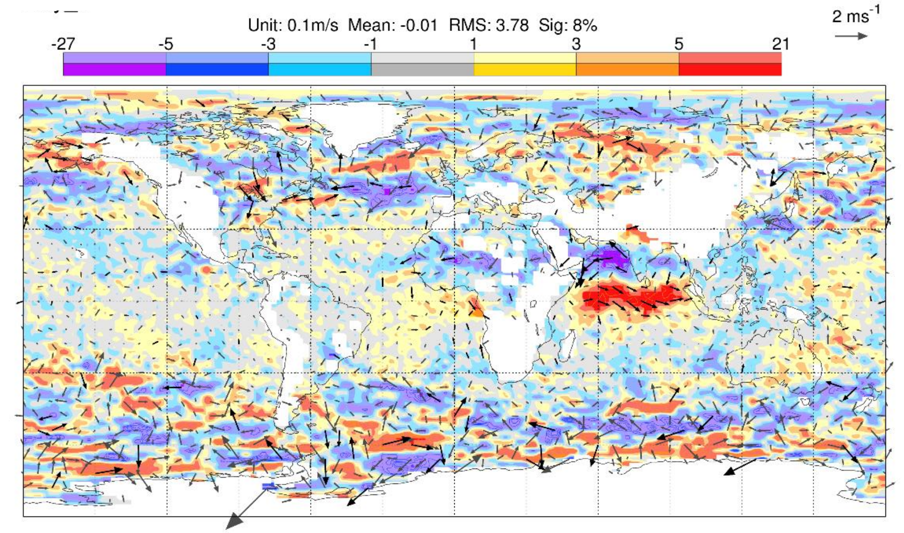
U 925 hPa – model bias at D+5

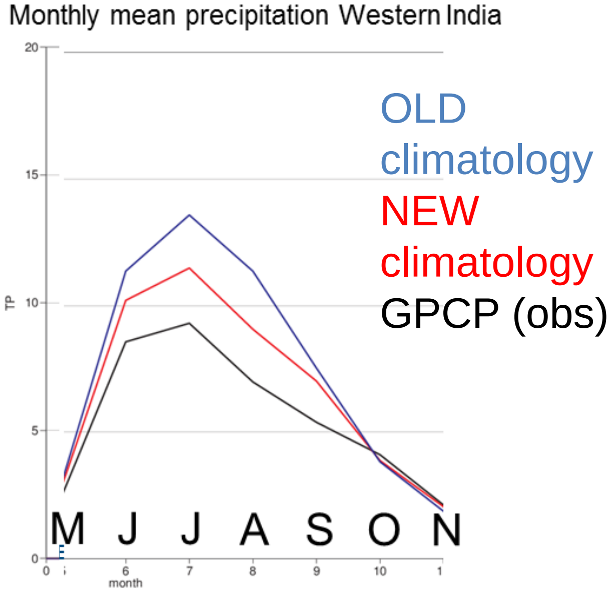




Too strong monsoon circulation in Indian Ocean in the model leads to too high precipitation over west India.

U 925 hPa – change in model bias

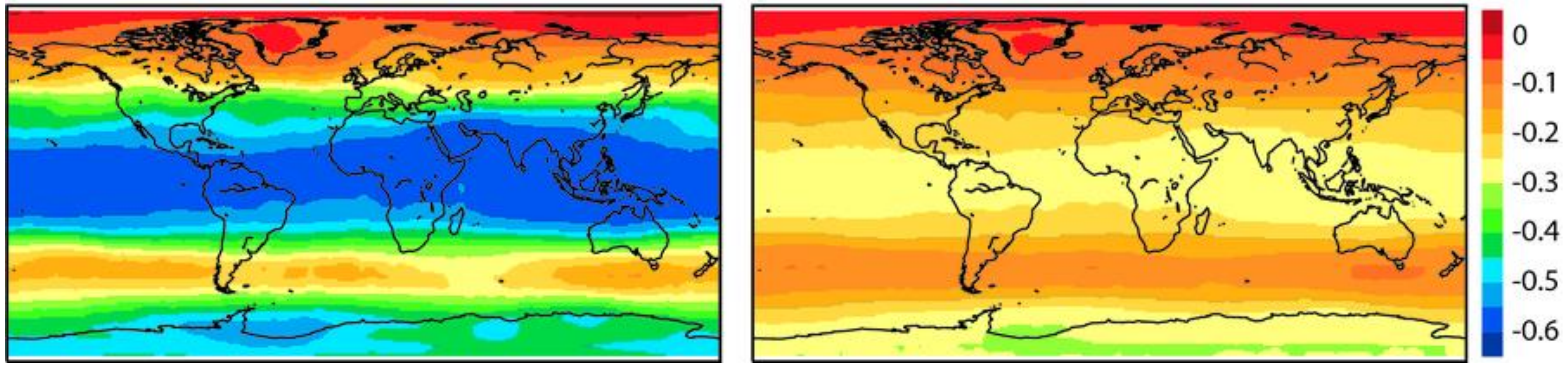




Revised aerosols affect the circulation and reduce the bias both in the wind circulation and in the precipitation amounts in Summer

Benefit of AC for NWP: Variable CO2 in radiance assimilation

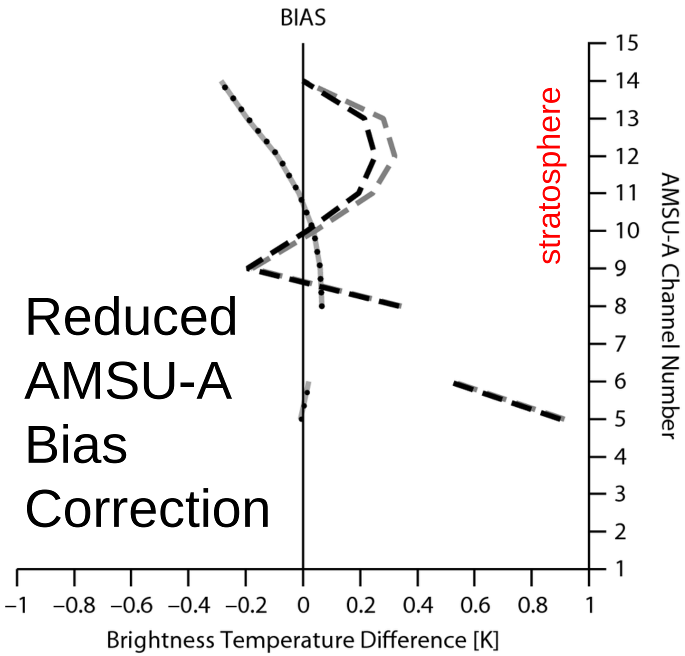
Reduced AIRS and IASI Bias Correction



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

Benefit of AC for NWP: Example of link between wind and tracer

Model equations

$$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}=\nu\frac{\partial^2 u}{\partial x^2}$$

$$\frac{\partial q}{\partial t}+u\frac{\partial q}{\partial x}=0$$

u = u(x,t) = wind over periodic domain [0,L]
q = q(x,t) = passive tracer
ν = diffusion coef.
$\delta u, \delta q$ = perturbations
$\delta' u, \delta' q$ = adjoint variables

Tangent linear equations:

$$\frac{\partial \delta u}{\partial t}+u\frac{\partial \delta u}{\partial x}+\delta u\frac{\partial u}{\partial x}=\nu\frac{\partial^2 \delta u}{\partial x^2}$$

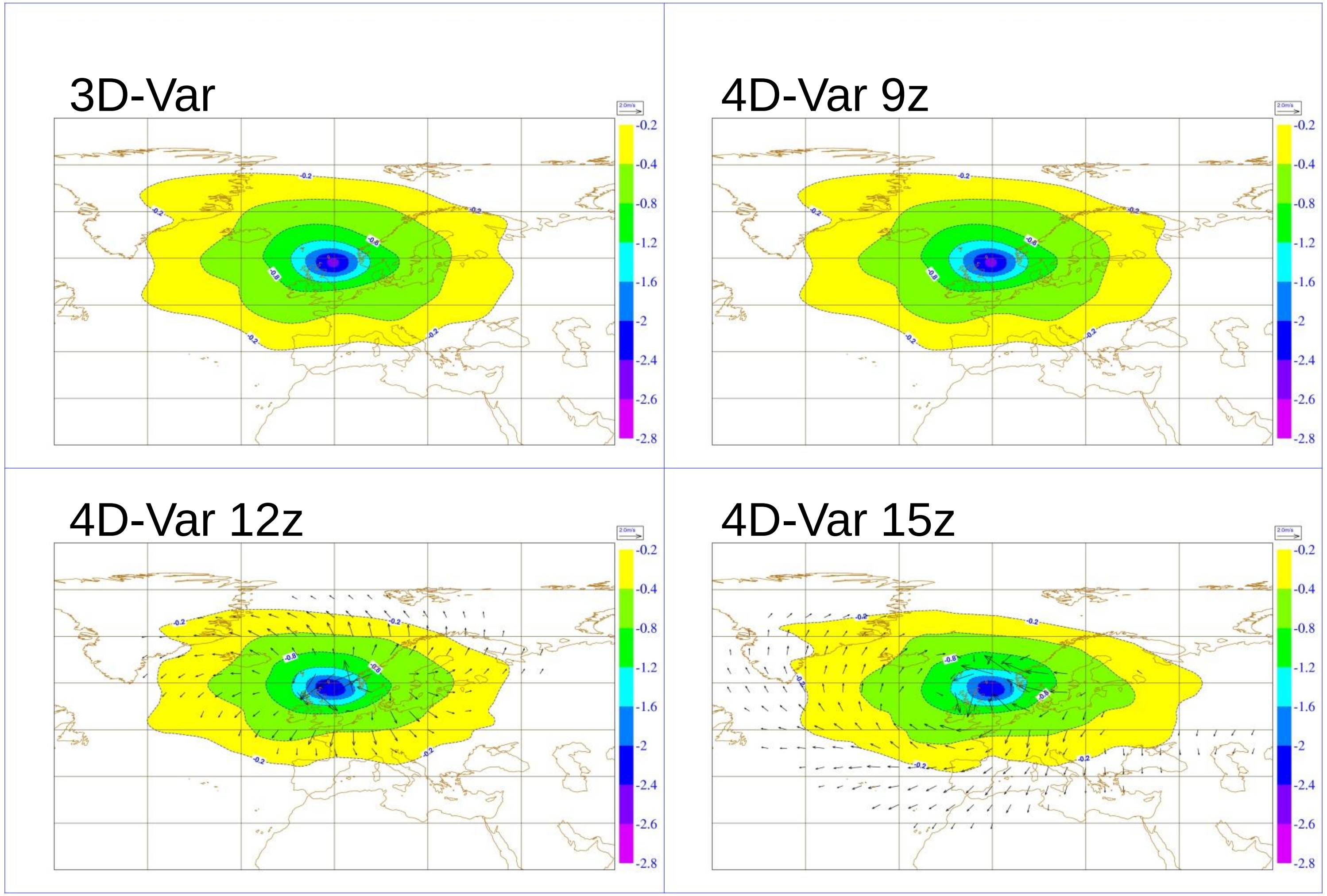
$$\frac{\partial \delta q}{\partial t}+u\frac{\partial \delta q}{\partial x}+\delta u\frac{\partial q}{\partial x}=0$$

Adjoint equations:

$$-\frac{\partial \delta' u}{\partial t}-u\frac{\partial \delta' u}{\partial x}+\frac{\partial u}{\partial x}\delta' u-\nu\frac{\partial^2 \delta' u}{\partial x^2}+\delta' q\frac{\partial q}{\partial x}=0$$

$$-\frac{\partial \delta' q}{\partial t}-\frac{\partial (u\delta' q)}{\partial x}=0$$

Single observation experiments - Ozone and wind increments



Level 20,
≈ 30 hPa

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

Observation at T3: wind increments

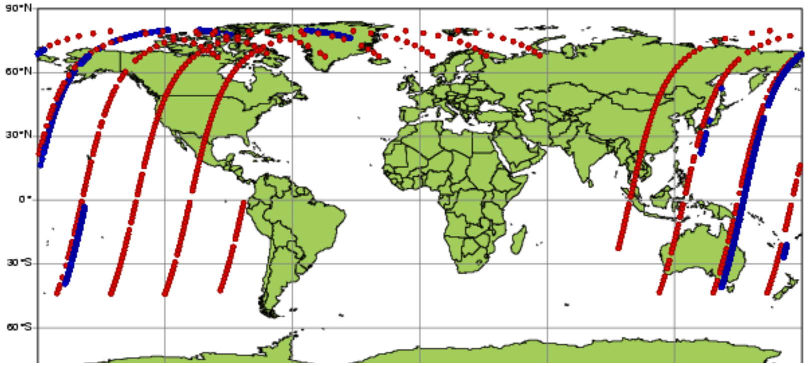
Observation at T6: wind increments

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

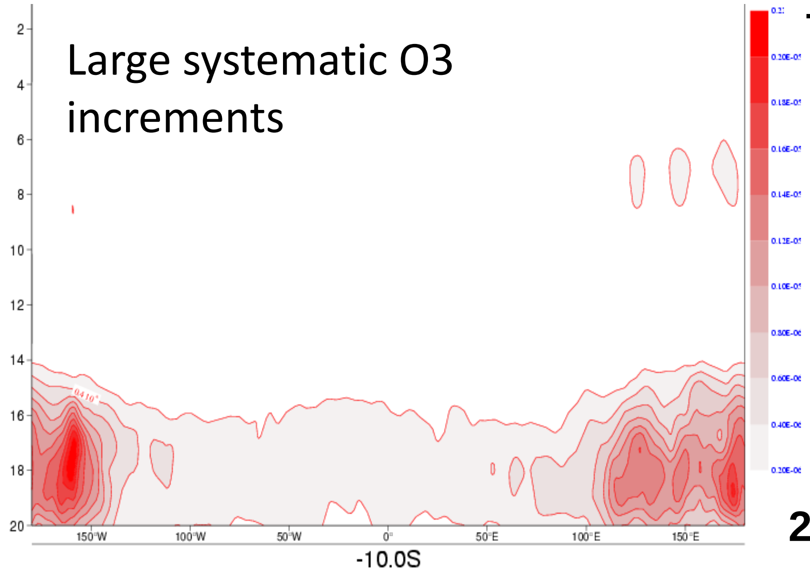


GOME 15-layer profiles (~15,000 per day)
SBUV 6-layer profiles (~1,000 per day)

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

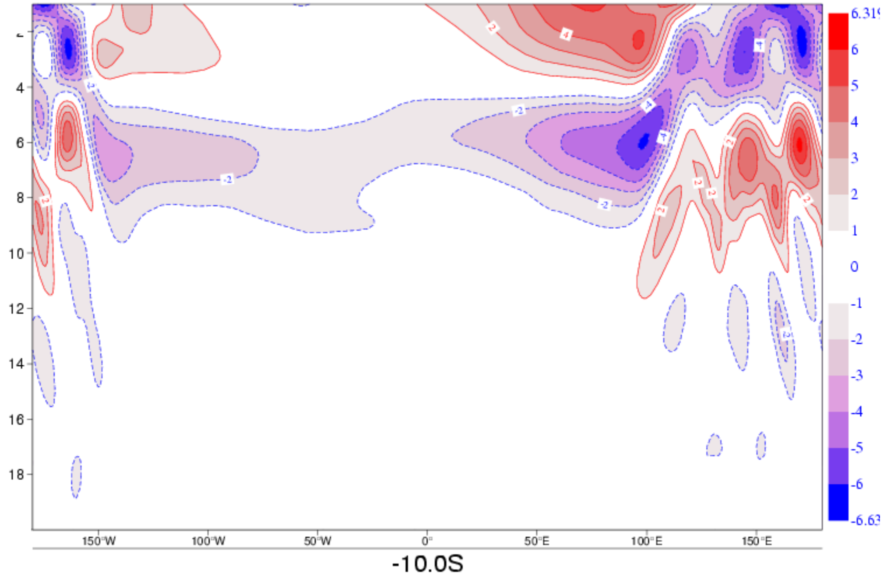
Ozone increments at 10S



1 hPa

20 hPa

Associated Temp increments



D. Dee

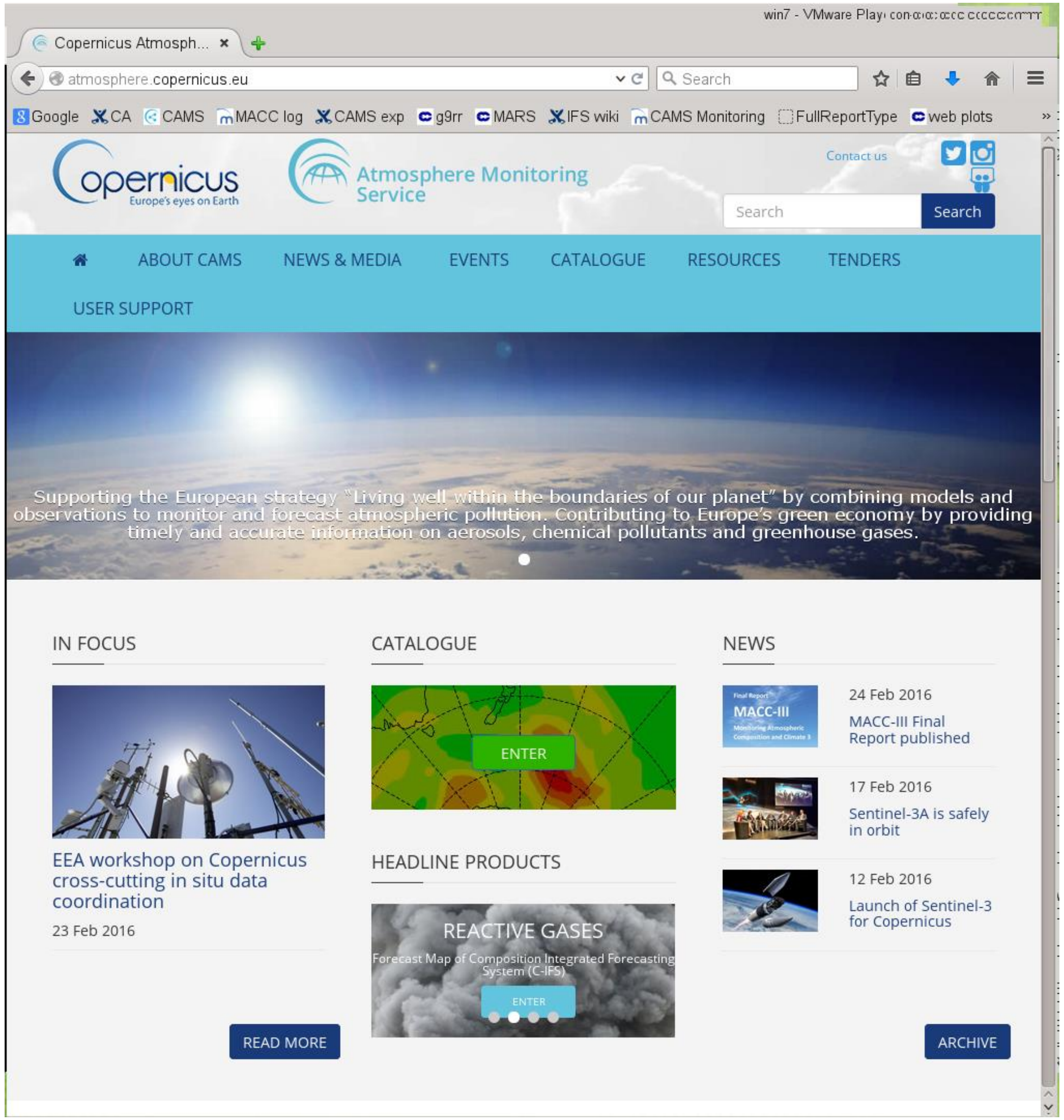
Summary

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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