Atmosphere Monitoring

Assimilation of Atmospheric Composition

Antje Inness,

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O v e r v i e w

1. Introduction
2. Challenges for atmospheric composition data assimilation
3. Observations of atmospheric composition
4. Aerosol data assimilation
5. Conclusions

1. Introduction

- Environmental and health concern - up to 7 million premature deaths per year (WHO) because of air pollution
- Important to provide air quality forecasts
- Not principally different from meteorological DA but several new challenges
- Interaction of atmospheric composition (AC) and NWP
  - Feedback on dynamics via radiation scheme (ozone, aerosols)
  - Precipitation and clouds (aerosols)
  - Satellite observations influenced by aerosols and trace gases
  - Hydrocarbon (Methane) oxidation is water vapour source
  - Assimilation of AC data can have impact on wind field

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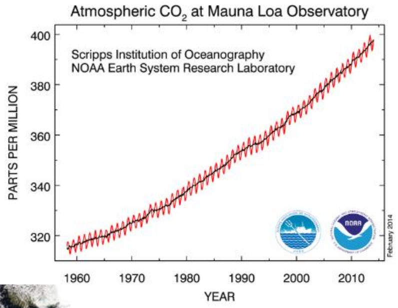
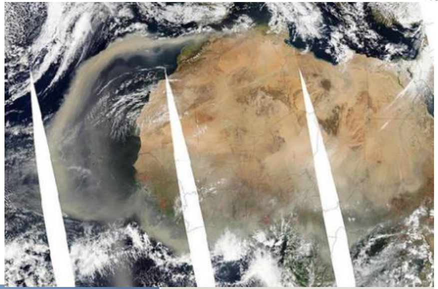
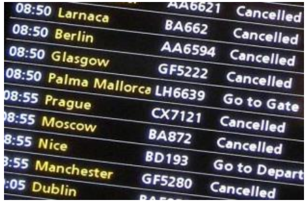
Examples of Atmospheric composition







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Composition in IFS

- Over the last decade IFS has been extended with modules for atmospheric composition (aerosols, reactive gases, greenhouse gases)
- GEMS -> MACC -> CAMS (Copernicus Atmosphere Monitoring Service) projects
- At first a "Coupled System", now composition fully integrated into IFS
- Data assimilation of AC data to provide best possible IC for subsequent forecasts
- AC benefits from online integration and high temporal availability of meteorological fields
- CAMS provides daily analyses and 5-day forecasts of atmospheric composition in NRT

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CAMS service provision

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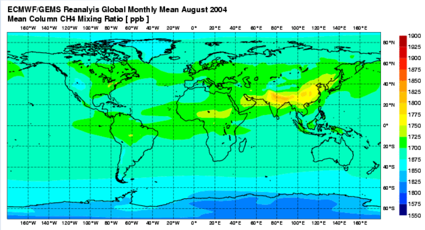
Retrospective

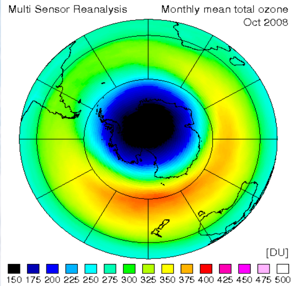
Daily (NRT)

Reanalysis

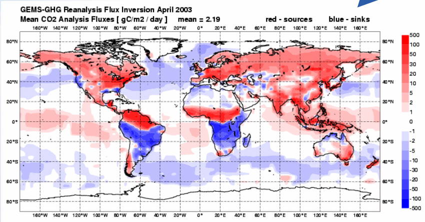
2003 onwards



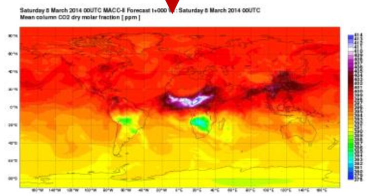
Ozone records



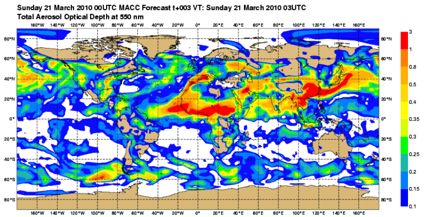
Flux Inversions



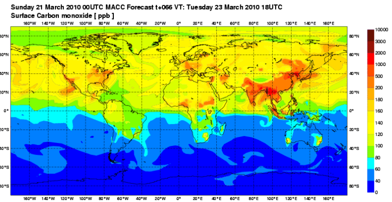
GHG



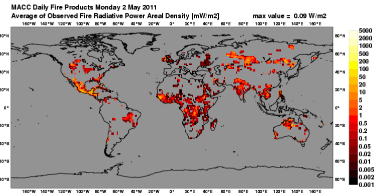
Aerosols



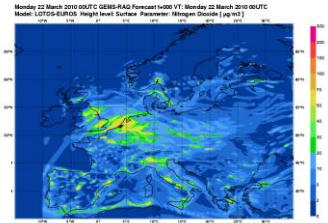
Global Pollution



Fires



Air quality



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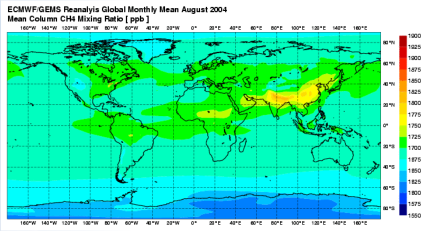
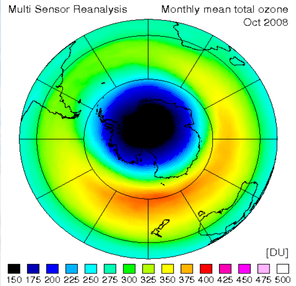
CAMS service provision

Retrospective

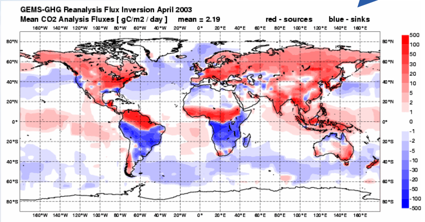
Reanalysis



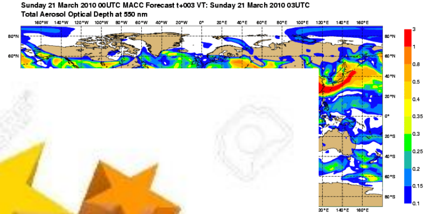
Ozone records

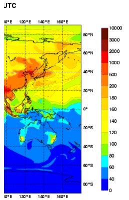


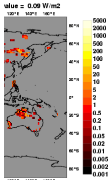
Flux Inversions

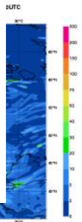


Daily (NRT)









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CAMS NRT data assimilation system

Extra information:
- Emissions (e.g. GFAS)
- Fluxes

Chemistry solvers included in IFS
e.g. TM5 (CB05)
54 species, 126 reactions
photolysis, dry and wet deposition
(no TL + AD of chemistry)

IFS control variables

CHEM: O3, NO2, SO2, CO, HCHO

AER: single or dual control variables (total or fine & coarse mode aerosol mixing ratio)

GHG: CO2, CH4

Meteorological variables

Aerosol model with 12 bins (no TL or AD)

GHG fields

Observations
- Observation operators
- Bias correction
- Background error statistics

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2. Challenges for atmospheric composition data assimilation

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Challenges

- Quality of NWP depends predominantly on initial state
- AC modelling depends on initial state (lifetime) and surface fluxes
- Large parts of chemical system not sensitive to initial conditions because of chemical equilibrium, but dependent on model parameters (e.g. emissions, deposition, reaction rates,…)
- Data assimilation is challenging for short lived species (e.g. NO2)
- CTMs have larger biases than NWP models
- Most processes take place in boundary layer, which is not well observed from space
- Only a few species (out of 100+) can be observed
- Concentrations vary over several orders of magnitude
- Data availability
- More complex and expensive, e.g. atmospheric chemistry, aerosol physics

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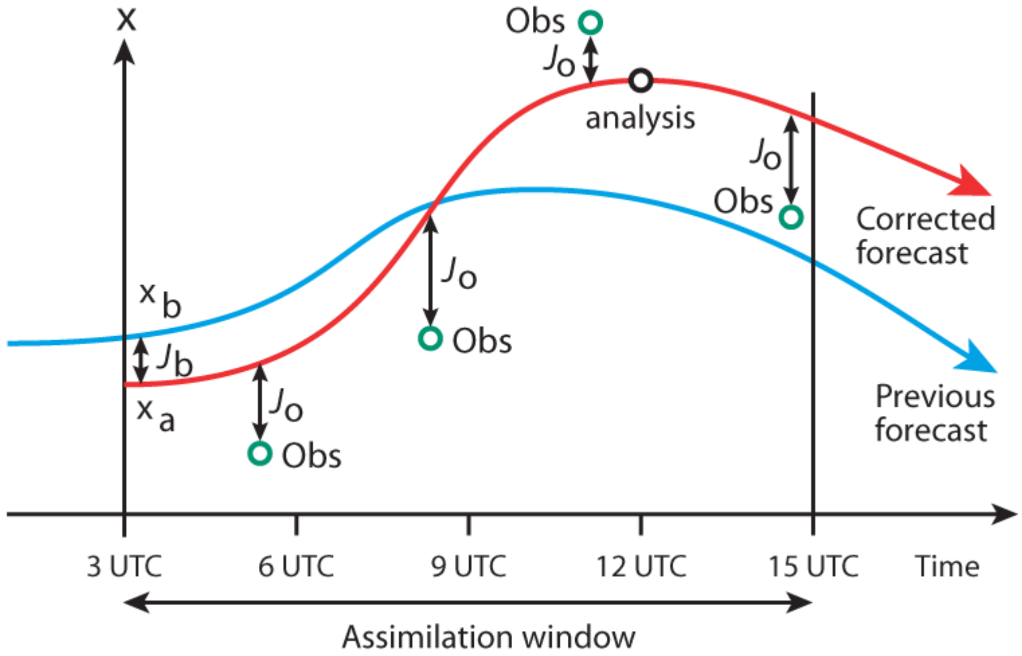
4D-Var



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

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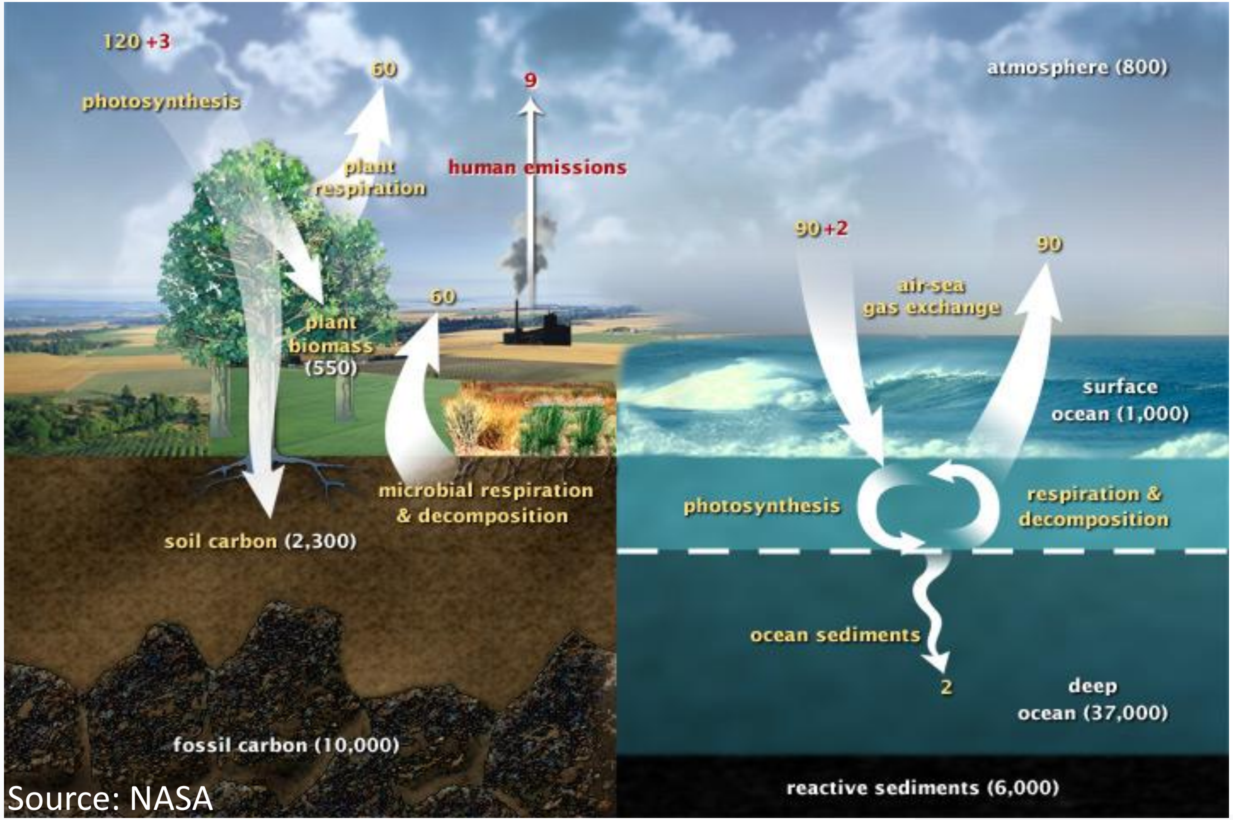
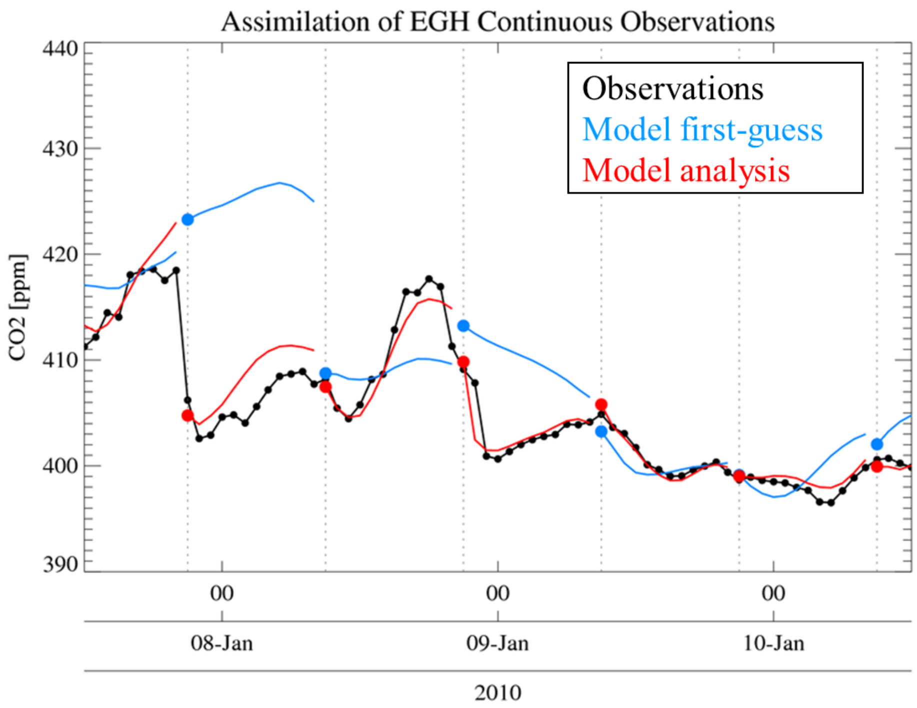
CO2 as an example



Source: NASA

Boundary condition problem – CO2



For atmospheric composition, the boundary conditions are very important (surface fluxes, emissions,…).

Credits: R. Engelen

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Emission Estimates

- Emissions are one of the major uncertainties in modelling (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 “modelled” 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)
- Emissions can be included in the control vector and adjusted together with concentrations (e.g. Hanea et al. 2004; Elbern et al. 2007; Miyazaki et al. 2012)

Emission Processes

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- Combustion related (CO, NOx, SO2, VOC, CO2)
  - fossil fuel combustion
  - biofuel combustion
  - vegetation fires (man-made and wild fires)
- Fluxes from biogeochemical processes (VOC, CH4, CO2, Pollen):
  - biogenic emissions (plants, soils, oceans)
  - agricultural emissions (incl. fertilisation)
- Fluxes from wind blown dust and sea salt (from spray)
- Volcanic emissions (ash, SO2, HBr …)
- In CAMS we use GFAS fire emissions (Kaiser et al. 2012), MACCity anthropogenic emissions (Granier et al. 2011) and Megan biogenic emissions (Guenther et al. 2006)
- Biomass burning accounts for ~ 30% of total CO and NOx emissions, ~10% CH4

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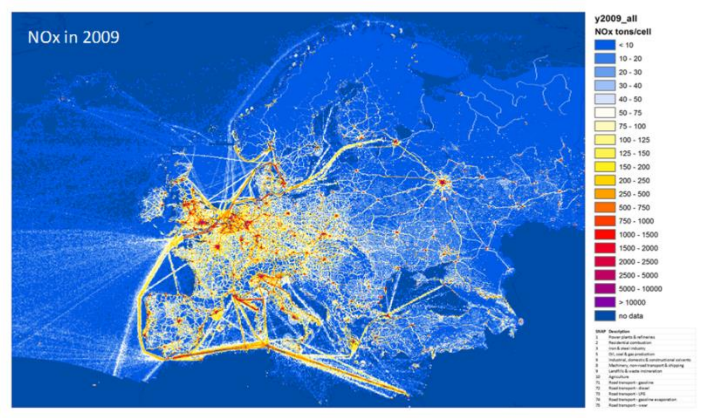
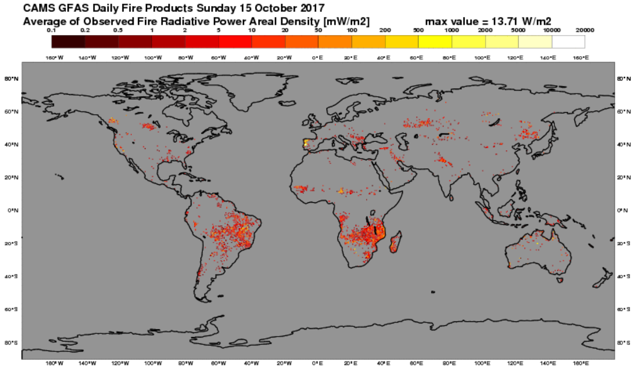
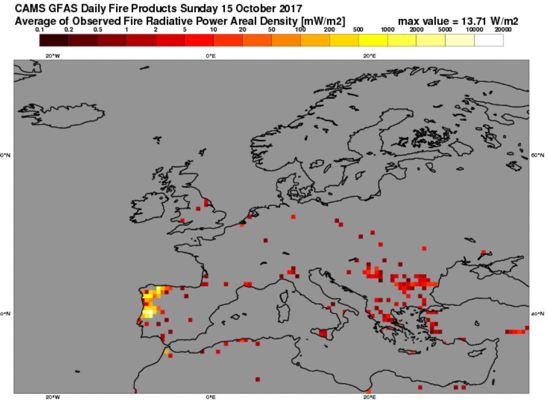
Emission Examples

TNO European anthropogenic Nox emissions



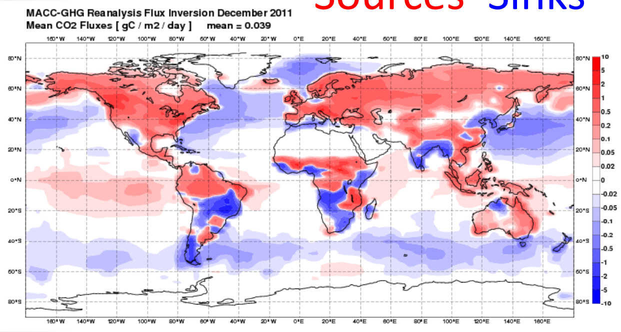


GFAS 15 October 2017



CO2 fluxes

Sources Sinks



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Importance of emissions (Russian fires 2010)

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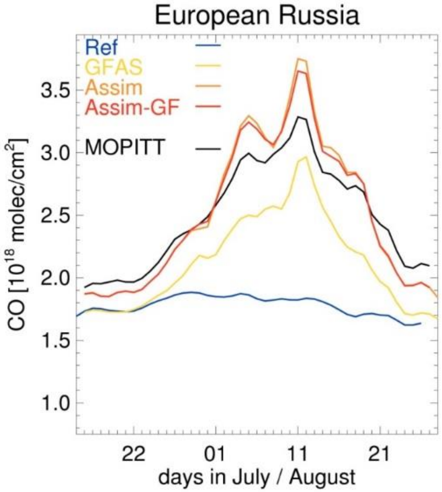
Huijnen et al. 2012 (ACP)

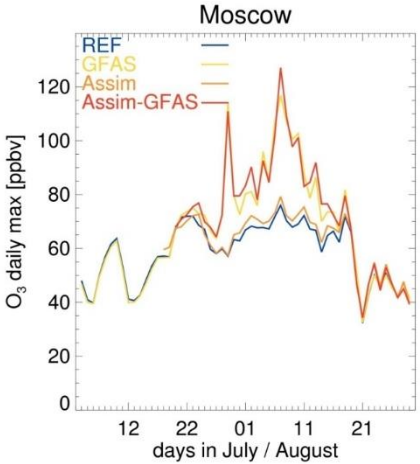
Total column CO

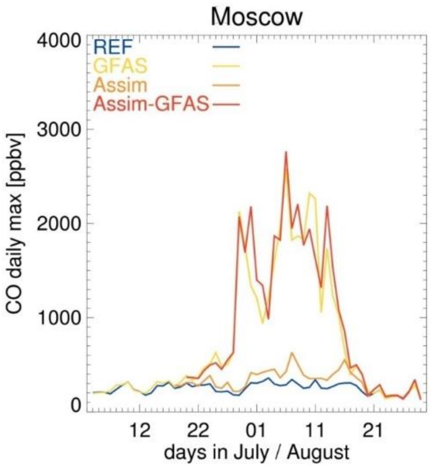


- Assimilation of IASI TCCO leads to improved fit to MOPITT TCCO
- TCCO from **Assim** and **Assim-GFAS** are very similar

GFAS emissions are needed to get peak in **surface concentrations** in **GFAS** and **Assim-GFAS**

Daily maximum surface O3 and CO





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Importance of fire emissions on tropospheric NO2

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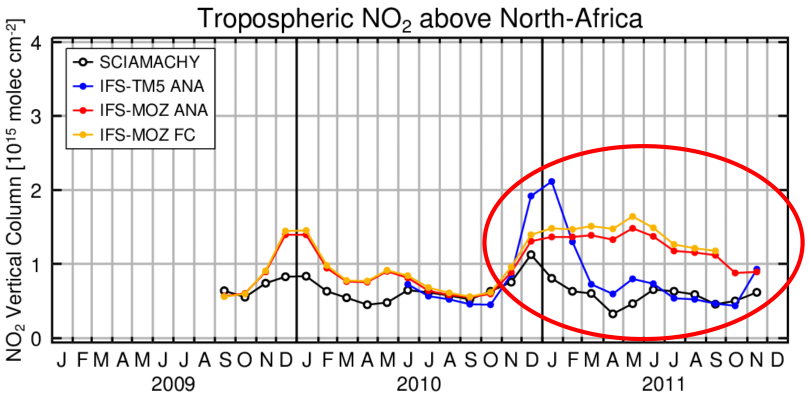
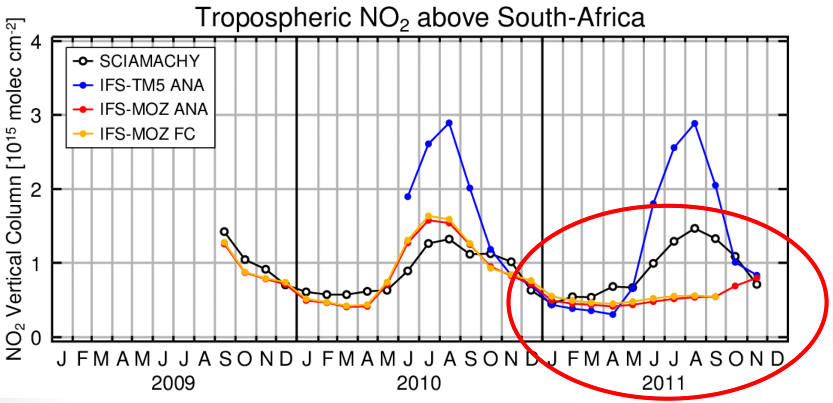


GFAS emissions for January used by mistake in IFS-MOZ during 2011



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Impact of anthropogenic emissions: CO Bias - GAW Europe timeseries

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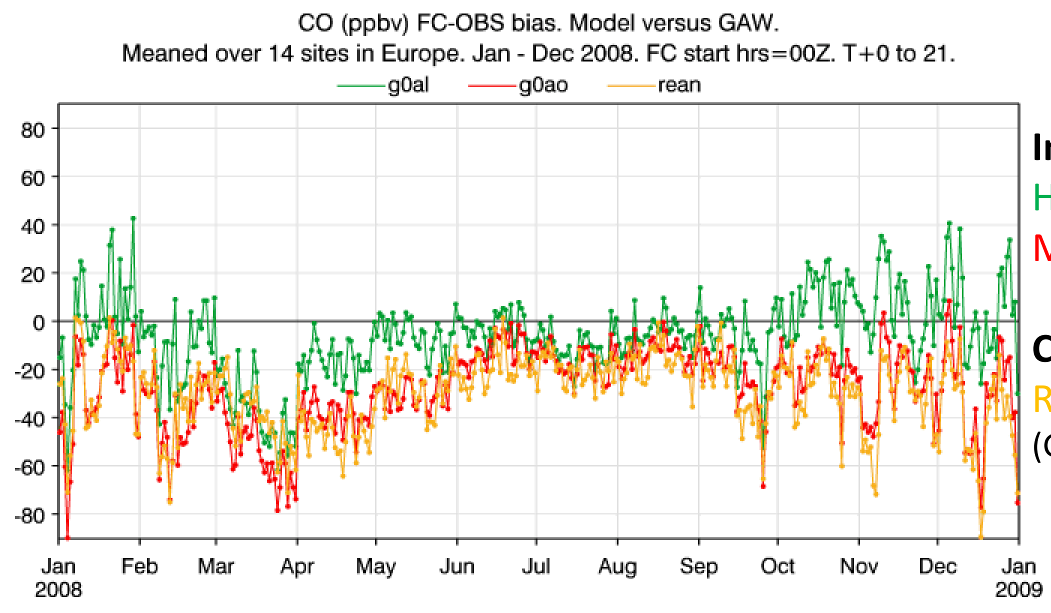

Integrated chemistry:
HTAP emissions
MACCity emissions

Coupled system:
Reanalysis (MACCity)
(GFAS used in all runs)

Choice of emissions data set has large impact on surface concentrations

J. Flemming

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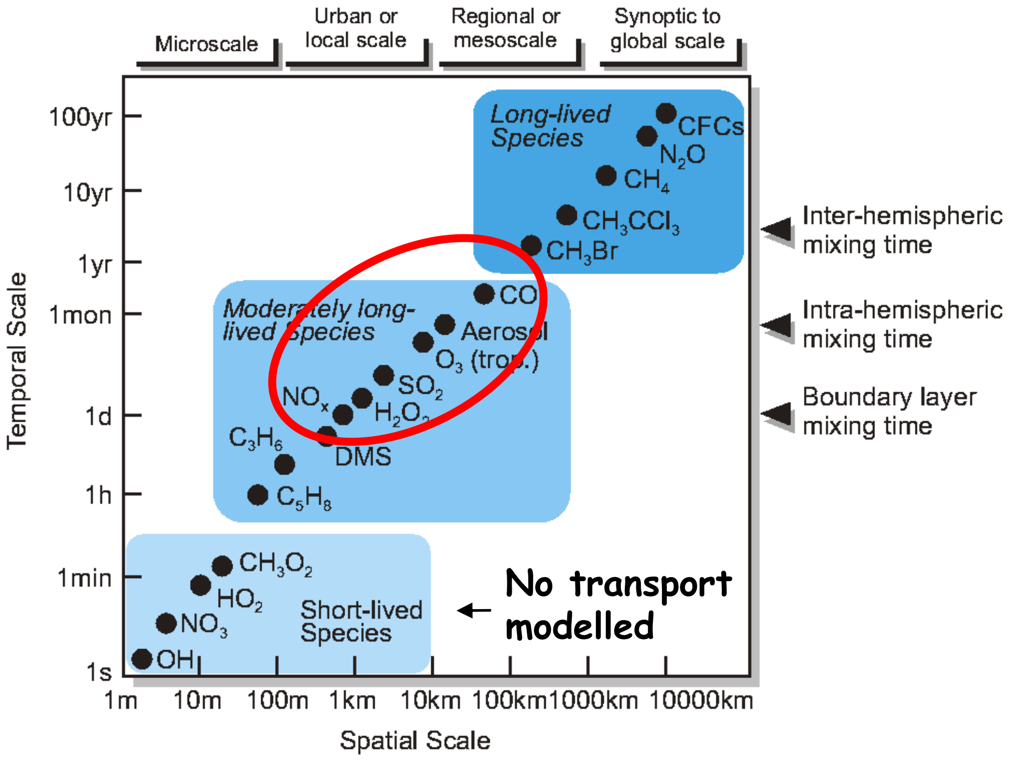
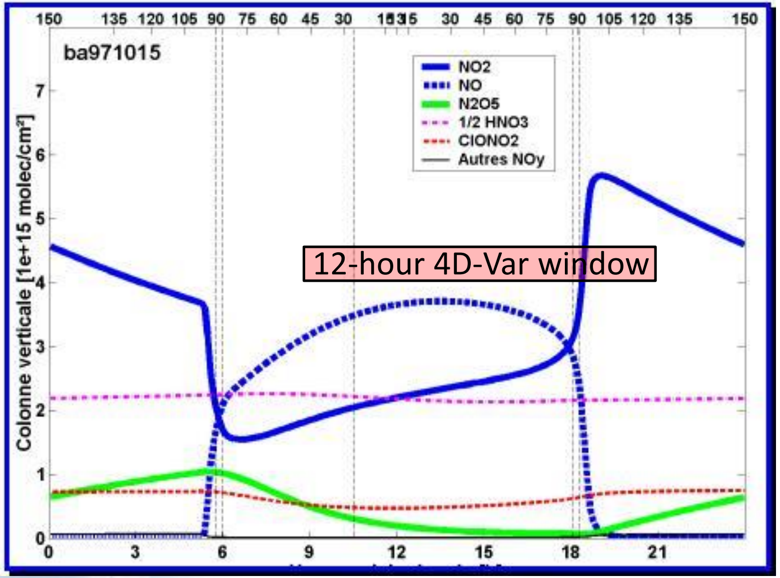
Chemical Lifetime vs. Spatial Scale



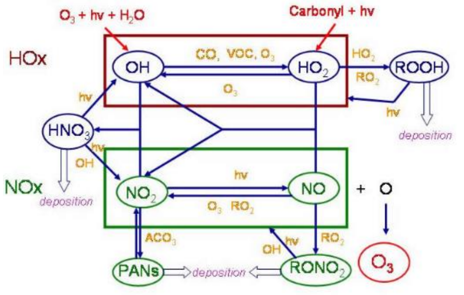
After Seinfeld and Pandis [1998]

NO_2 data assimilation



Credits: J-C Lambert (BIRA)

- Satellite observations of NO_2 are not straightforward to assimilate.
- Fast chemistry makes it difficult to treat it as an initial value problem without a proper chemistry adjoint, because of the strong diurnal cycle.



Credit: BIRA/IASB

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

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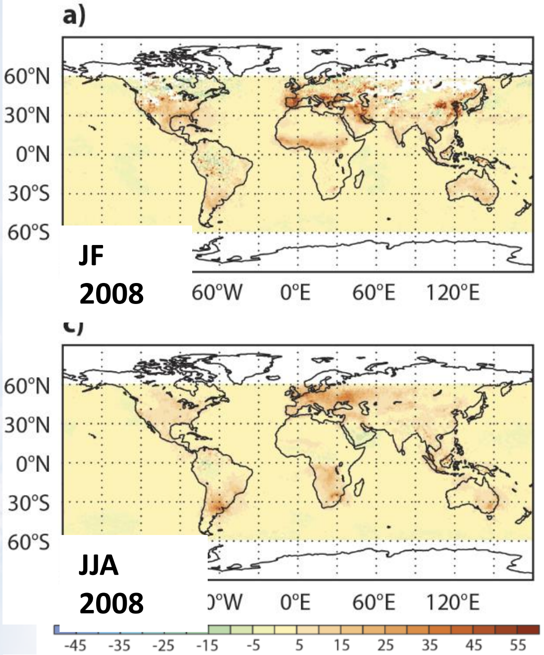
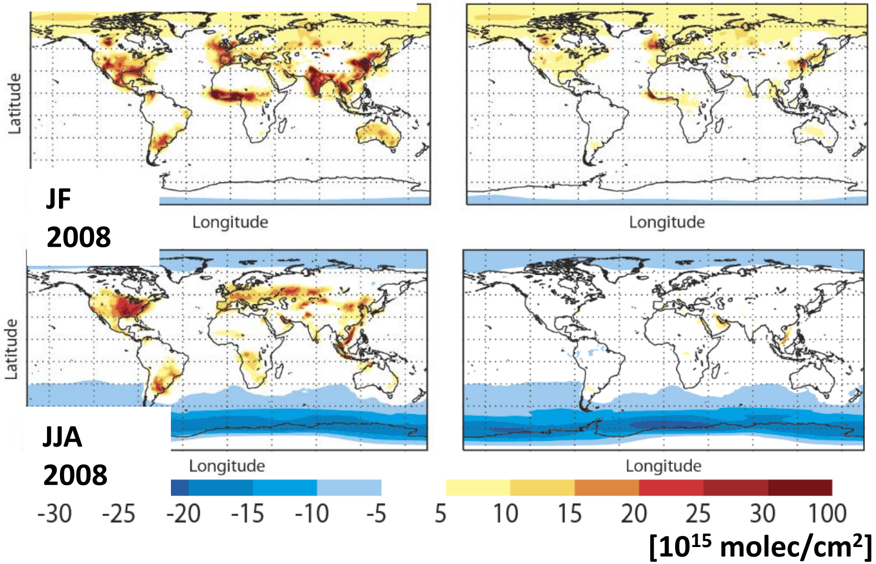
OMI NO2 analysis increment [%]



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 would be more beneficial to adjust emissions (instead of IC)

Inness et al. 2015

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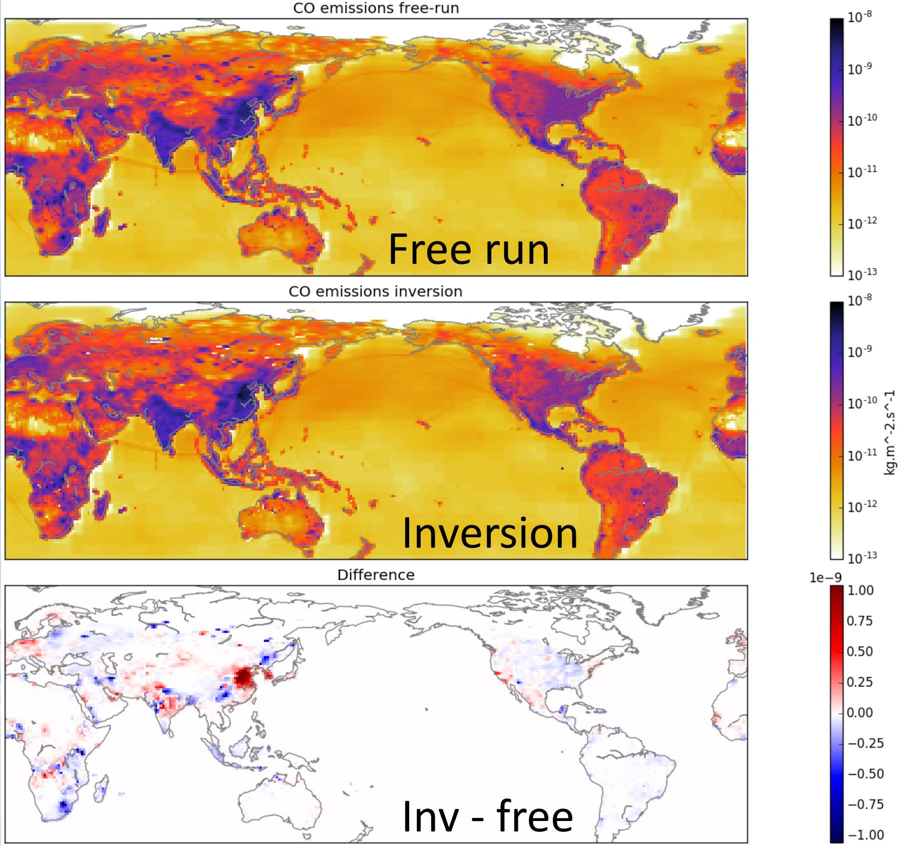
CO inversion

Ensemble mean of emissions



- First tests with 25 members EDA (T159) with perturbed emissions
- LinCO scheme (Cariolle and Massart, 2014)
- MOPITT and IASI TCCO assimilated
- May-June 2017
- Linear regression between the increments and emissions at each outer loop for each ensemble member

  ➡ Emission increment

- Looks promising
- Validation with independent data to follow

Credits: J. Barré

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3. Observations of atmospheric composition

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Satellite observations

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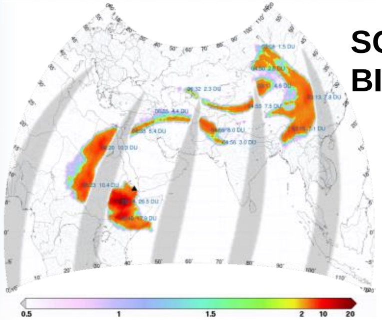
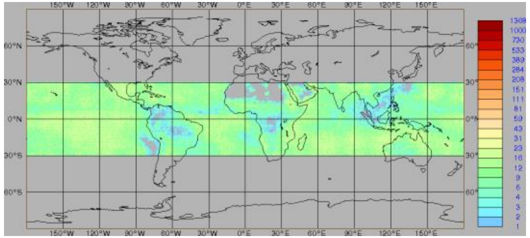
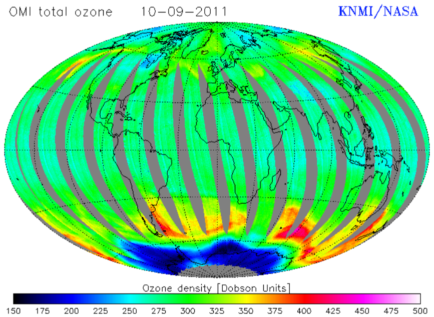
SO_2, GOME-2, SACS, BIRA/DLR/EUMETSAT



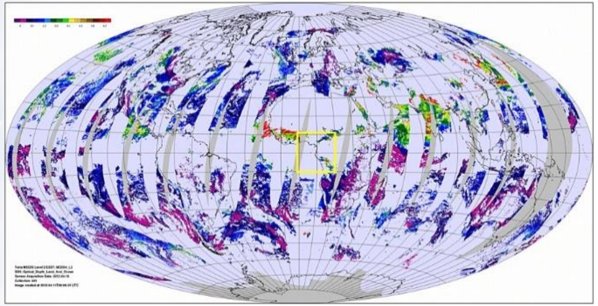
CH_4, IASI, LMD



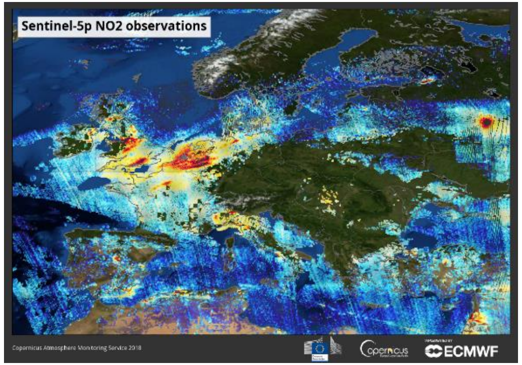
O_3, OMI, KNMI/NASA



Aerosol Optical Depth, MODIS, NASA



NO_2, TROPOMI, KNMI/ESA



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

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Issues with observations

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- AC Satellite retrievals
- Little or no vertical information from satellite observations. Total or partial columns retrieved from radiation measurements. Weak or no signal from boundary layer.
- Fixed overpass times and daylight conditions only (UV-VIS) -> no daily maximum/cycle
- Global coverage in a few days (LEO); often limited to cloud free conditions; fixed overpass time.
- Retrieval errors can be large; small scales not resolved
- Averaging kernels important
- AC in-situ observations
- Sparse (in particular profiles)
- Limited or unknown spatial representativeness

Reactive gases data availability in CAMS NRT system

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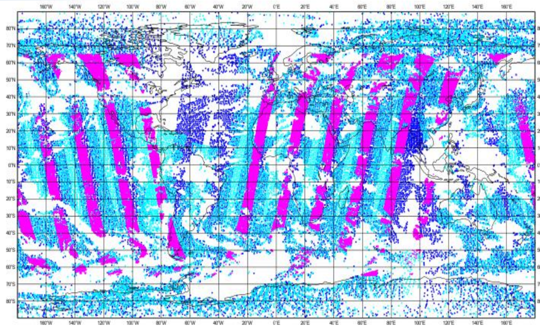
CO

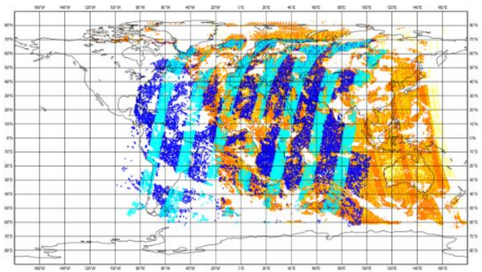


IASI Metop-A

IASI Metop-B

MOPITT TERRA

Tropospheric NO2



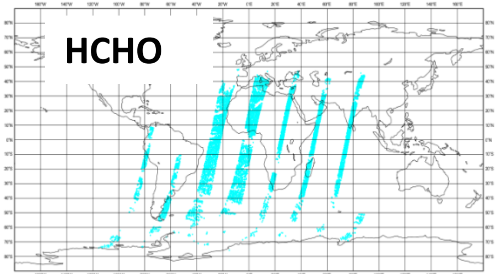
OMI AURA

TROPOMI S5P

GOME-2 Metop-A

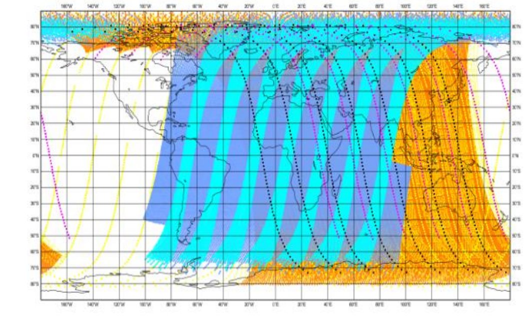
GOME-2 Metop-B

HCHO



GOME-2 Metop-A

O3



GOME-2 Metop-A

GOME-2 Metop-B

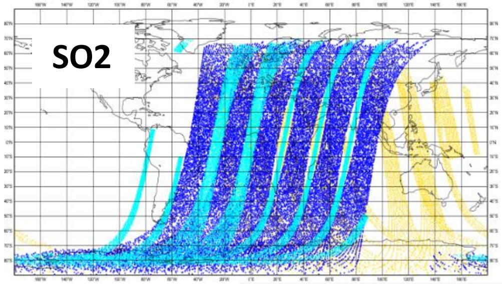
OMI, MLS AURA

SBUV/2 NOAA-19

TROPOMI S5P

OMPS SNPP

SO2



OMI AURA

GOME-2 Metop-A

GOME-2 Metop-B

assimilated

monitored

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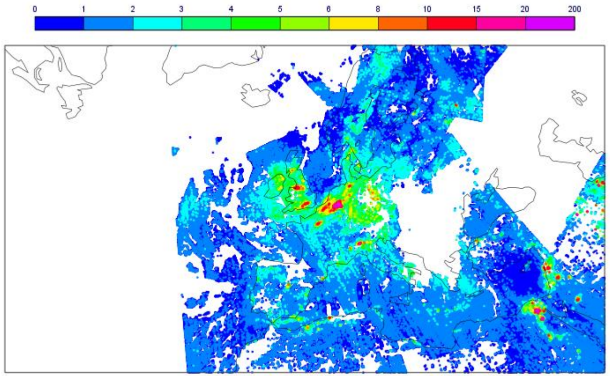
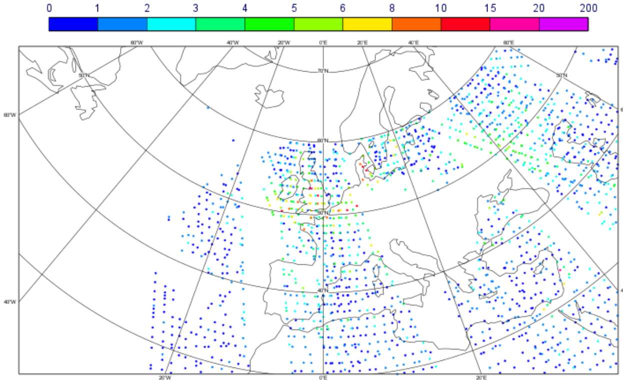
New data: Tropomi (S5P) data coverage

27 June 2018

TROPOMI (ESA, full resolution)

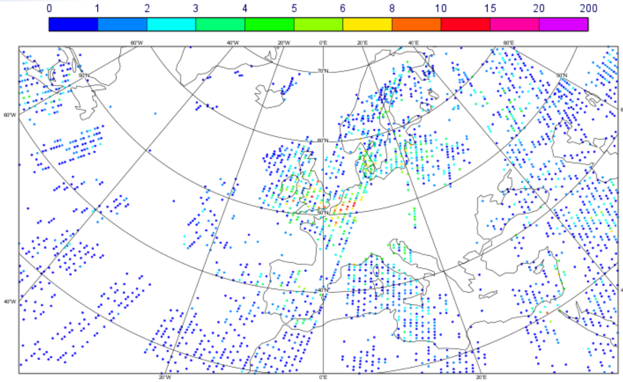


OMI (DOMINO-V2)

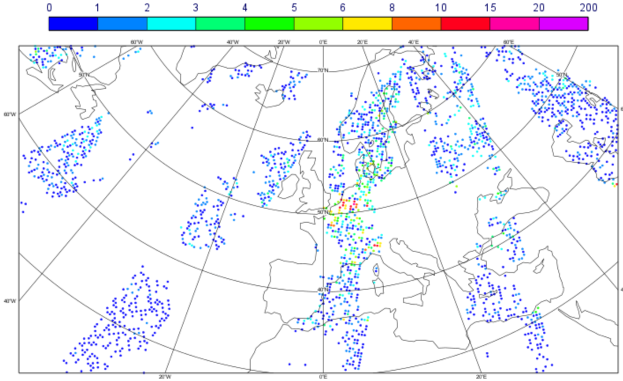


- GOME-2 and OMI thinned to $0.5^{o} \times 0.5^{o}$ and cloud cleared
- TROPOMI cloud cleared

GOME-2B (GDP v4.8)



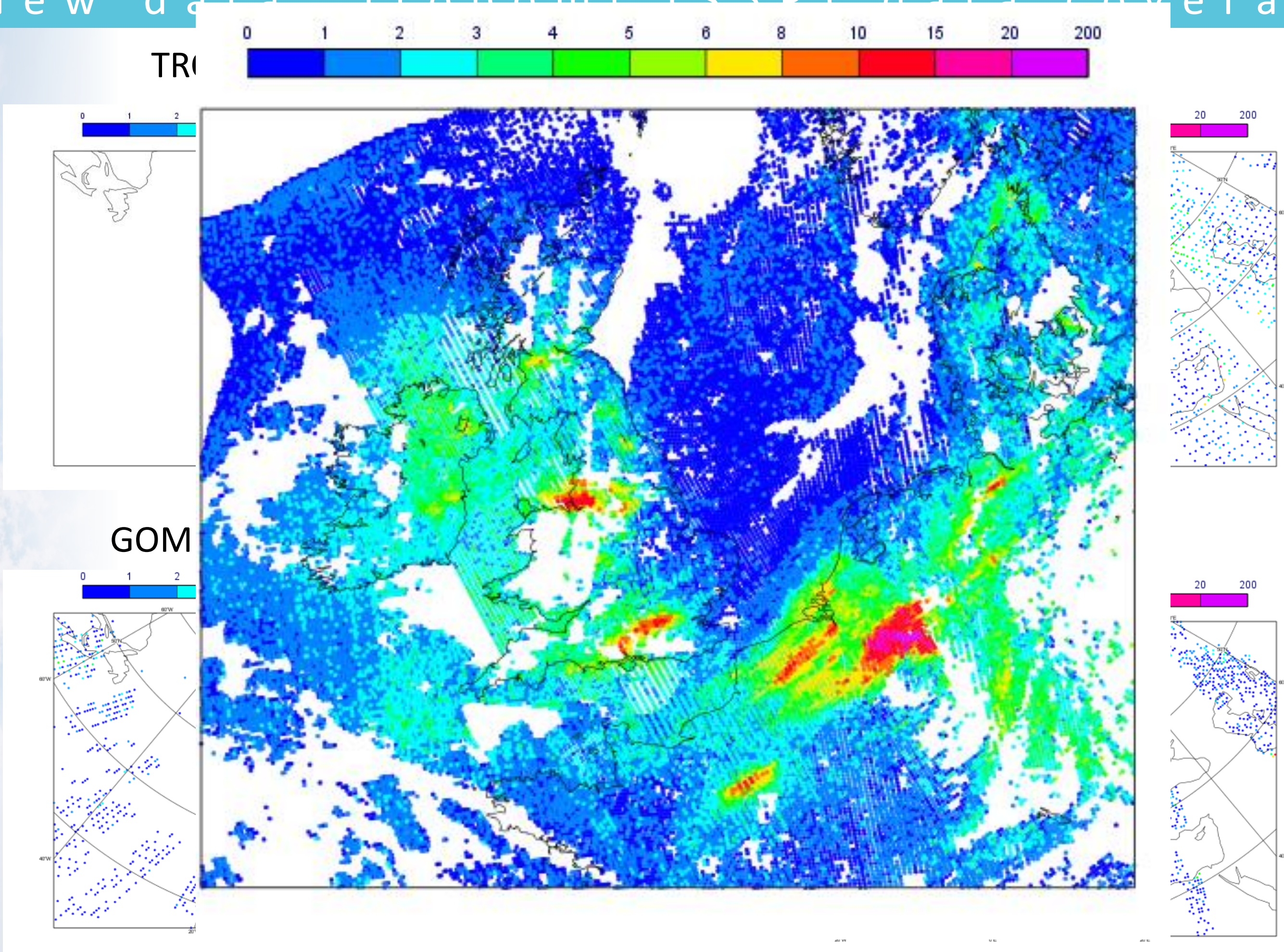
GOME-2A (GDP v4.8)



European Commission

New data: Tropomi (S5P) data coverage

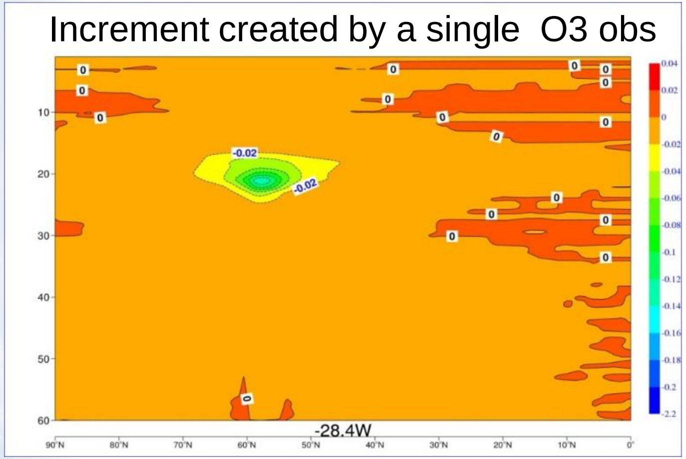
Atmosphere Monitoring



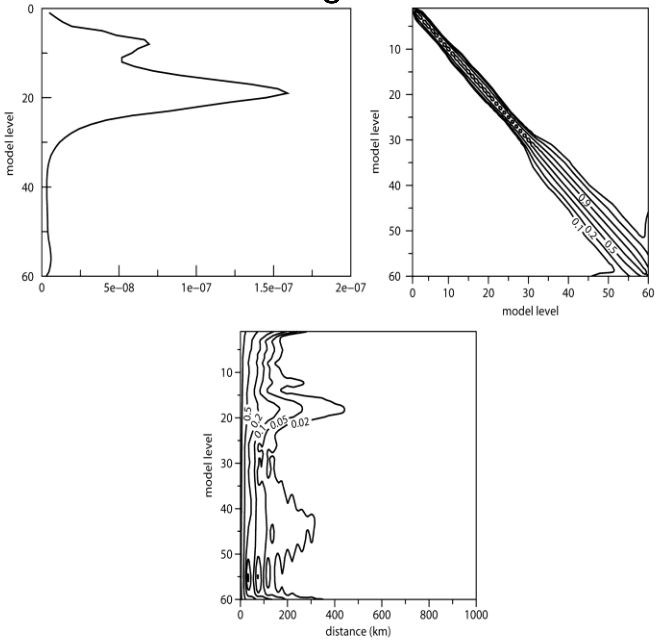
27 June 2018

- GOME-2 and OMI thinned to 0.5° x 0.5° and cloud cleared
- TROPOMI cloud cleared

Increment from a single TCO3 observation

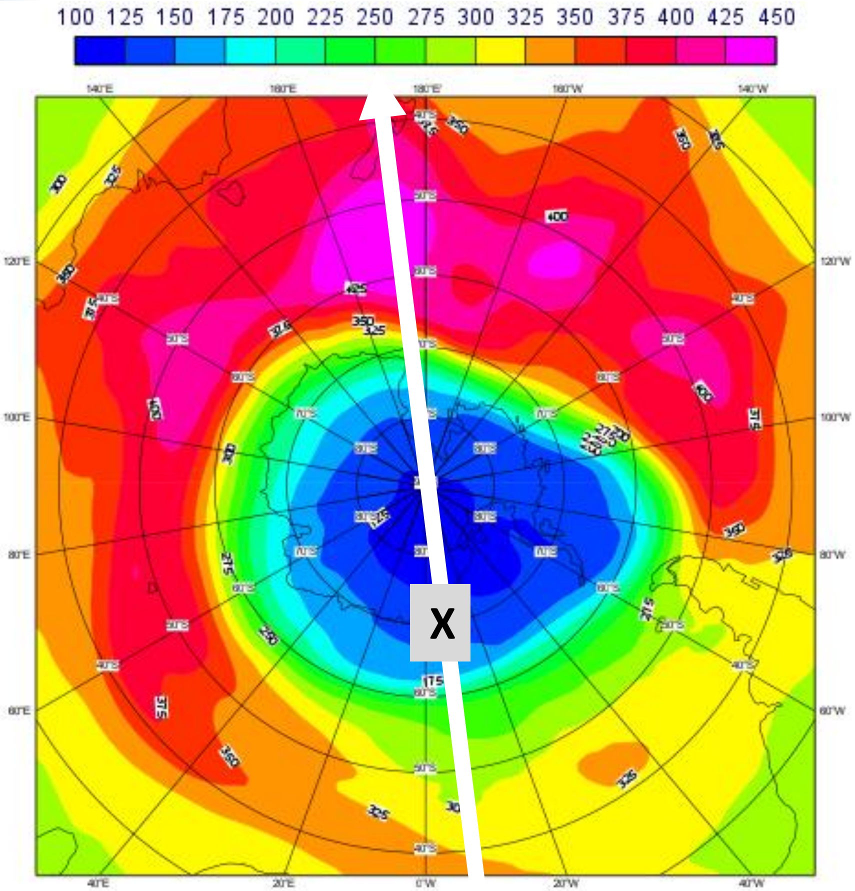


Ozone observation of 247 DU, 66 DU lower than background



- Maximum impact around L20 (~35 hPa)
- Profile data are important to obtain a good vertical analysis profiles

Ozone hole 4 October 2003



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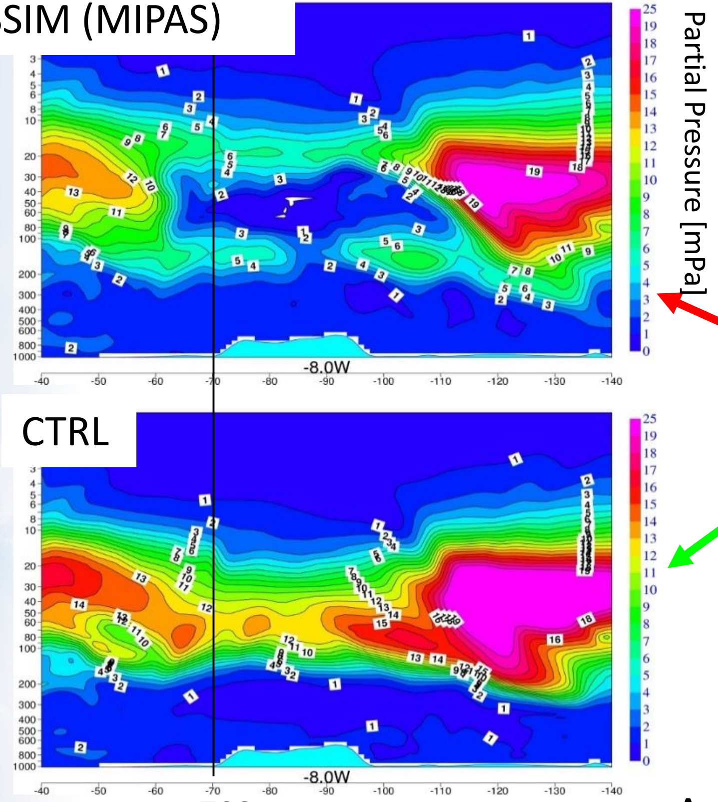
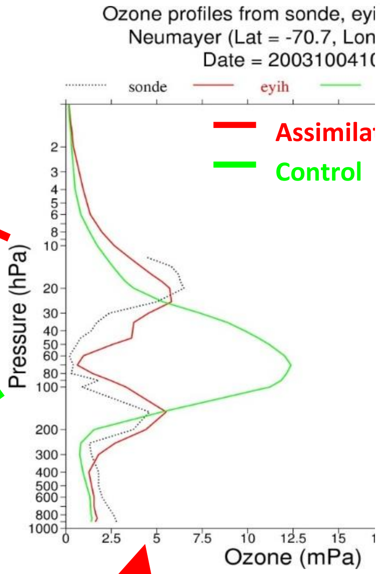
Ozone hole in GEMS reanalysis: Cross section along 8E over South Pole, 4 Oct 2003

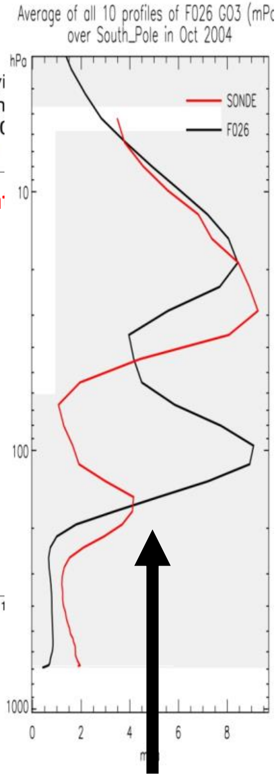
Atmosphere Monitoring

ASSIM (MIPAS)





Oct 2004



Assimilation **with profile data**

Assimilation **with total column data**

European Commission

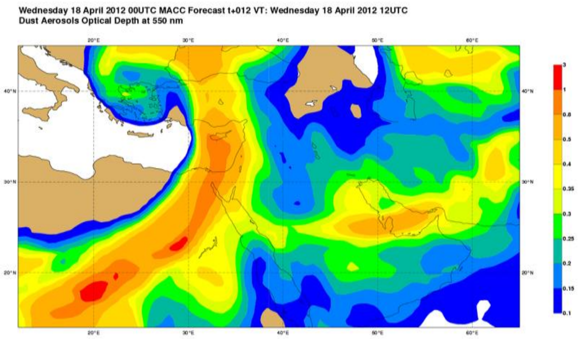
Atmosphere Monitoring

4. Aerosol data assimilation

4D-Var assimilation system for aerosols

Atmosphere Monitoring

- Aerosol assimilation is difficult because:
- There are numerous unknowns (depending on the aerosol model) and very little observations to constrain them
- The concentrations vary hugely with for instance strong plumes of desert dust in areas with very little background aerosol, which makes it difficult to estimate the background error covariance matrix



Aerosols in the IFS

Atmosphere Monitoring

- 12 aerosol-related prognostic variables:
  - 3 bins of sea-salt (0.03 – 0.5 – 0.9 – 20 μm)
  - 3 bins of dust (0.03 – 0.55 – 0.9 – 20 μm)
  - Black carbon (hydrophilic and –phobic)
  - Organic carbon (hydrophilic and –phobic)
  - SO_2 -> SO_4

- Physical processes include:
  - emission sources (some of which updated in NRT, i.e.fires),
  - horizontal and vertical advection by dynamics
  - vertical advection by vertical diffusion and convection
  - aerosol specific parameterizations for dry deposition, sedimentation, wet deposition by large-scale and convective precipitation, and
  - hygroscopicity (SS, OM, BC, SU)

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

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Aerosol assimilation in the IFS

- Assimilated observations are the 550nm MODIS (Aqua and Terra) Aerosol Optical Depths (AODs) over land and ocean and PMAp (Metop-A & -B) AOD 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
- Background error statistics were computed using forecast errors with the NMC method (48h-24h forecast differences).
- Observation errors are prescribed fixed values for MODIS/ given for PMAp
- Variational bias correction is applied to AOD
- Individual aerosol components are not well constrained

AOD data in CAMS NRT system, 20180201, 12z

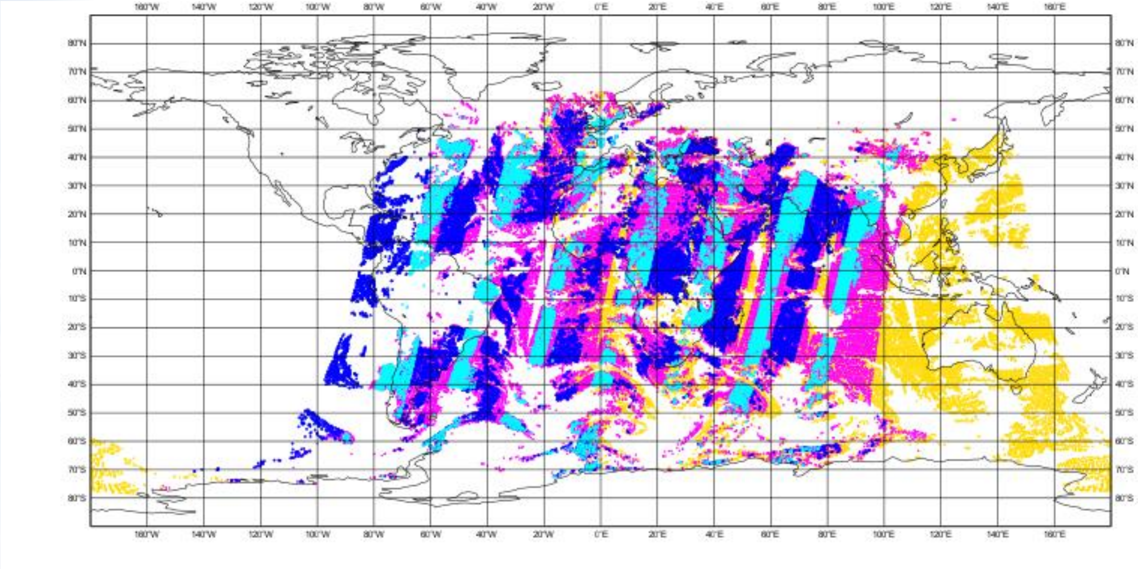
Atmosphere Monitoring

MODIS Aqua

MODIS Terra

PMAp Metop-B

PMAp Metop-A



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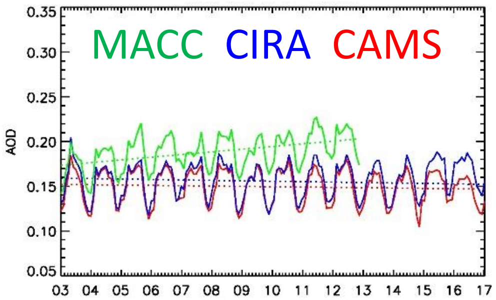
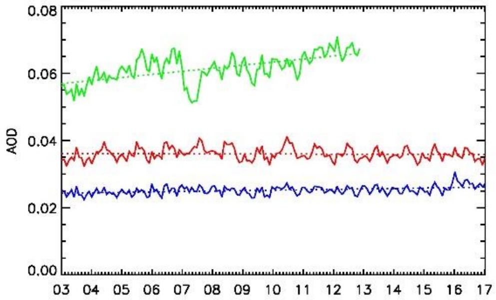
Aerosol Speciation from three reanalyes

Atmosphere Monitoring

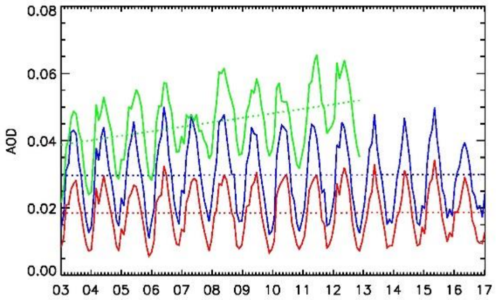
Total AOD



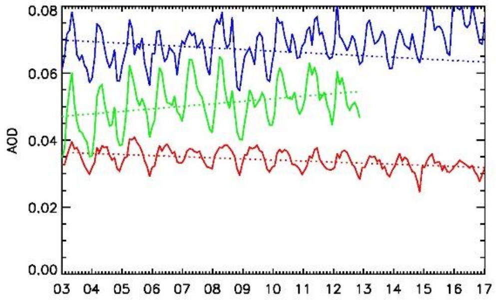
Sea Salt



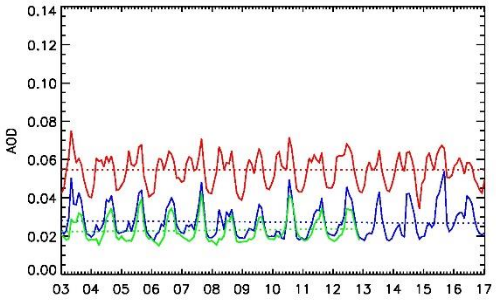
Dessert Dust



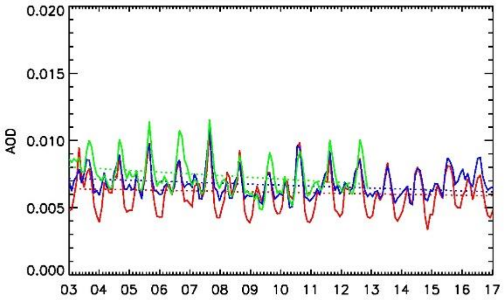
Sulphates



Organic Matter



Black Carbon



Even though total AOD in CIRA and CAMS is close there are considerable changes in the aerosol composition

J. Flemming

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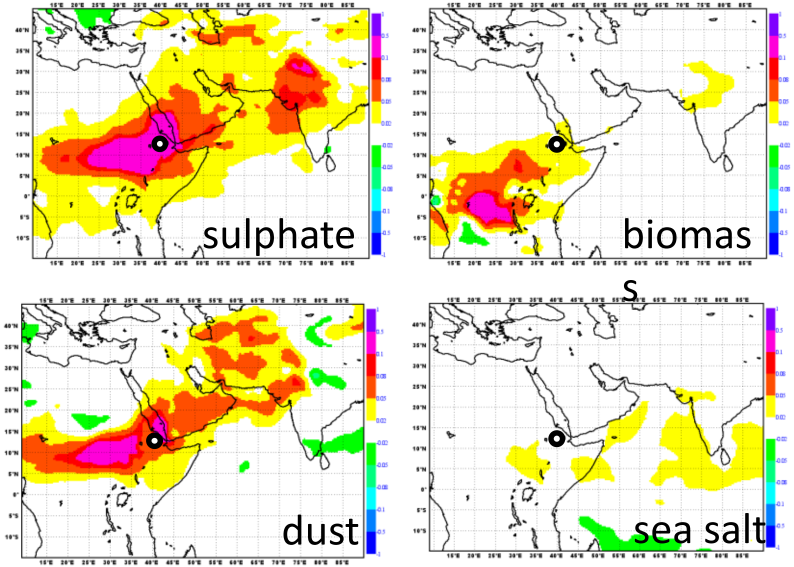
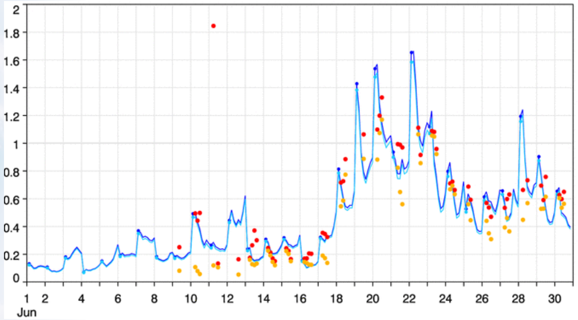
Example for wrong aerosol attribution

Eruption of the Nabro volcano in June 2011 put a lot of fine ash into the stratosphere.
This was observed by AERONET stations and the MODIS instrument.



ICIPE-Mbita - AERONET



MACC AOD analysis
AERONET total AOD
AERONET fine mode AOD

The MACC aerosol model did not contain stratospheric aerosol at this time, so the observed AOD was wrongly attributed to the available aerosol types.

Credits: A. Benedetti

5. Conclusions

Atmosphere Monitoring

- Atmospheric composition (AC) and weather interact
- IFS includes fields of atmospheric composition: Reactive gases, greenhouse gases, aerosols
- Modelling of AC expensive - includes many species with concentrations varying over several orders of magnitude
- AC forecasts benefit from realistic initial conditions (data assimilation) but likewise from improved emissions and models
- Extra challenges for DA of atmospheric composition compared to NWP
  - Additional information needed (emissions, deposition, reaction rates …)
  - Short lived species tricky
  - Species not constrained by assimilated observations (e.g. aerosols)
  - Resolution of observations often not adequate (vertical, horizontal, temporal)
- Potential benefits for NWP
- CAMS air quality forecasts and analyses are freely available from atmosphere.copernicus.eu
- New CAMS reanalysis of atmospheric composition (2003-2016) will be released next week