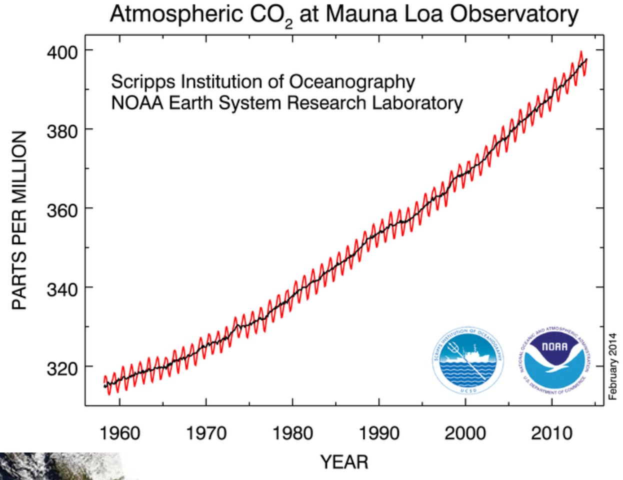
Data Assimilation of Atmospheric Composition

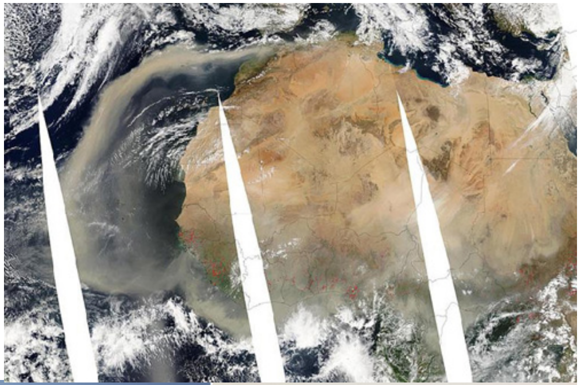
Antje Inness

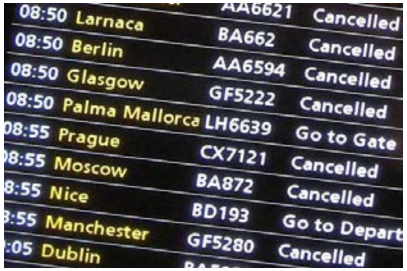
Contributions from: Angela Benedetti, Richard Engelen, Johannes Flemming and Sebastien Massart

ECMWF

Atmospheric composition







Outline

- Introduction
- Challenges for atmospheric composition DA
- Observations of atmospheric compositon
- Reactive gases assimilation
- Aerosol assimilation
- Concluding remarks

Introduction

- Environmental concern
- Expertise in data assimilation and atmospheric modelling
- Not principally different from meteorological DA but several new challenges
- Interaction atmospheric composition and NWP
  - Radiation triggered heating and cooling
  - Precipitation and clouds
  - Satellite data observations influenced by aerosols
  - Hydrocarbon (Methane) oxidation is water vapour source
  - Assimilation of atm. composition data can have impact on wind field

- **IFS has been extended to include chemically reactive gases (CO, O3, NO2, SO2, HCHO…), aerosols & greenhouse gases (CO2, CH4)**

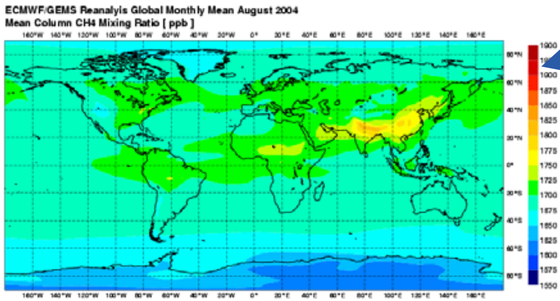
MACC Service Provision

Retrospective

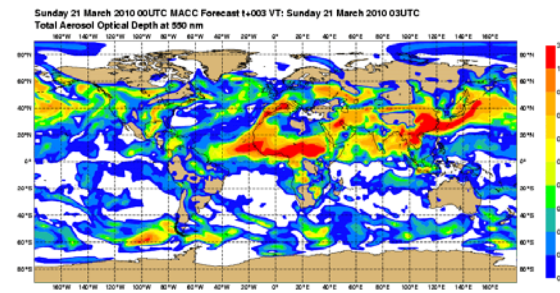
Daily (NRT)

Reanalysis

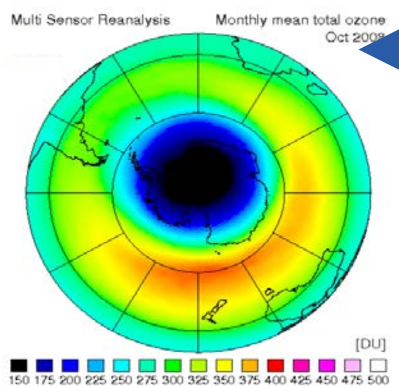
2003-2012



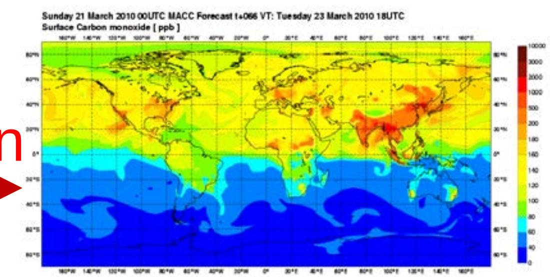
Aerosols



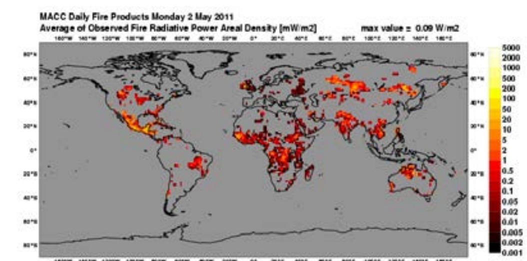
Ozone records



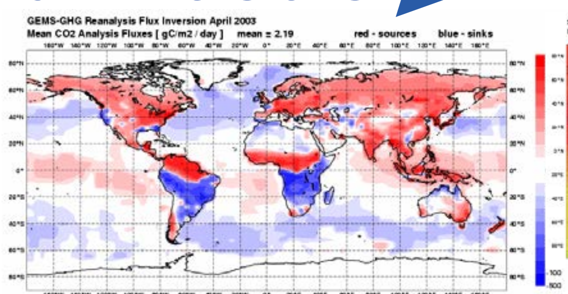
Global Pollution



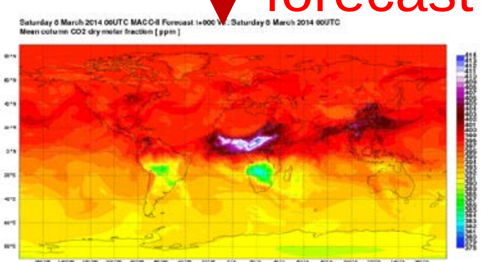
Fires



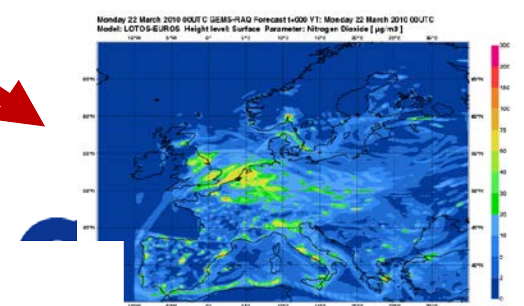
Flux Inversions



CO_2 forecast

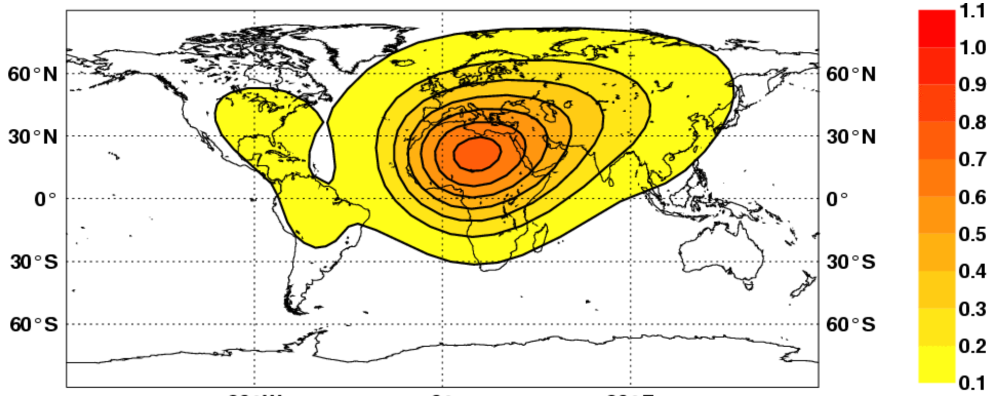


Air quality

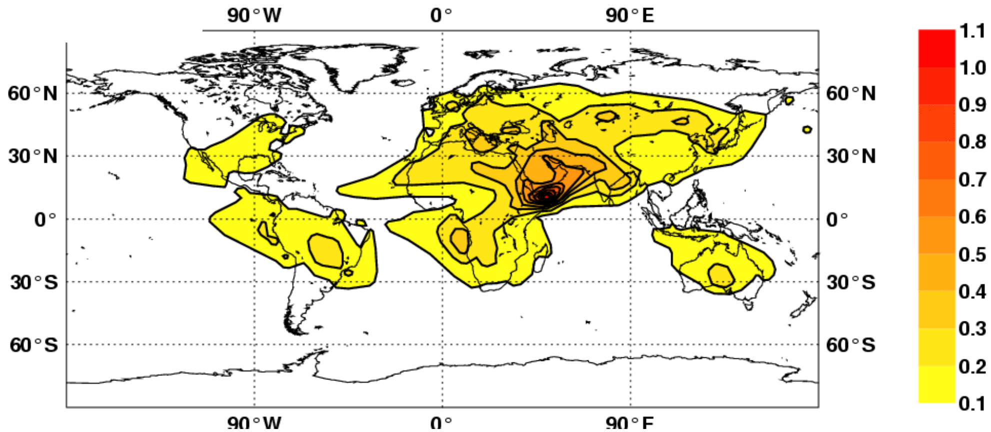


www.gmes-atmosphere.eu

Impact of Aerosol Climatology on NWP



26r1: Old aerosol (Tanre et al. 84 annually fixed)



26r3: New aerosol (June) Tegen et. al 1997

Change in Aerosol Optical Thickness Climatologies

Thickness at 550nm

Old aerosol dominated by Saharan sand dust

New: Reduction in Saharan sand dust & increased sand dust over Horn of Africa

J.-J. Morcrette
A. Tompkins

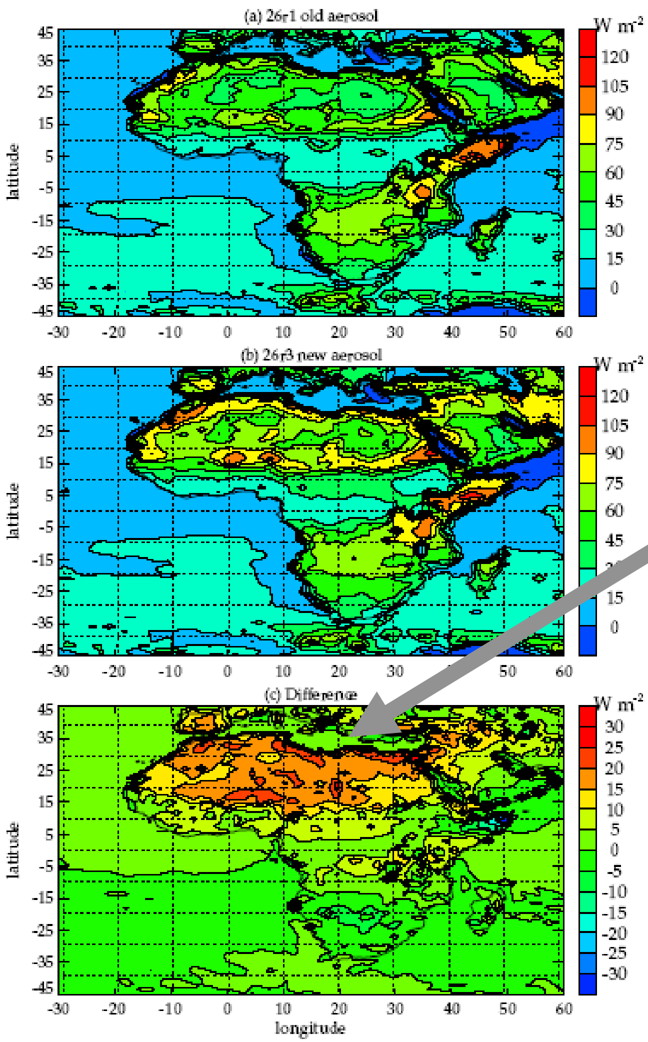
ECMWF

Impact of Aerosol Climatology on NWP

old

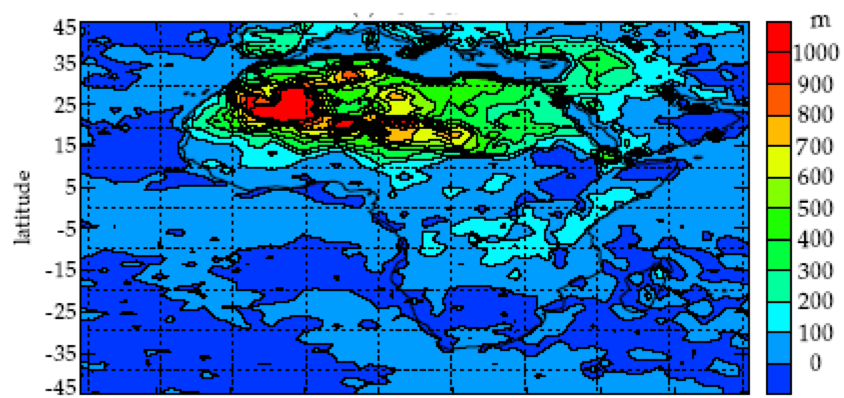
new

New-old



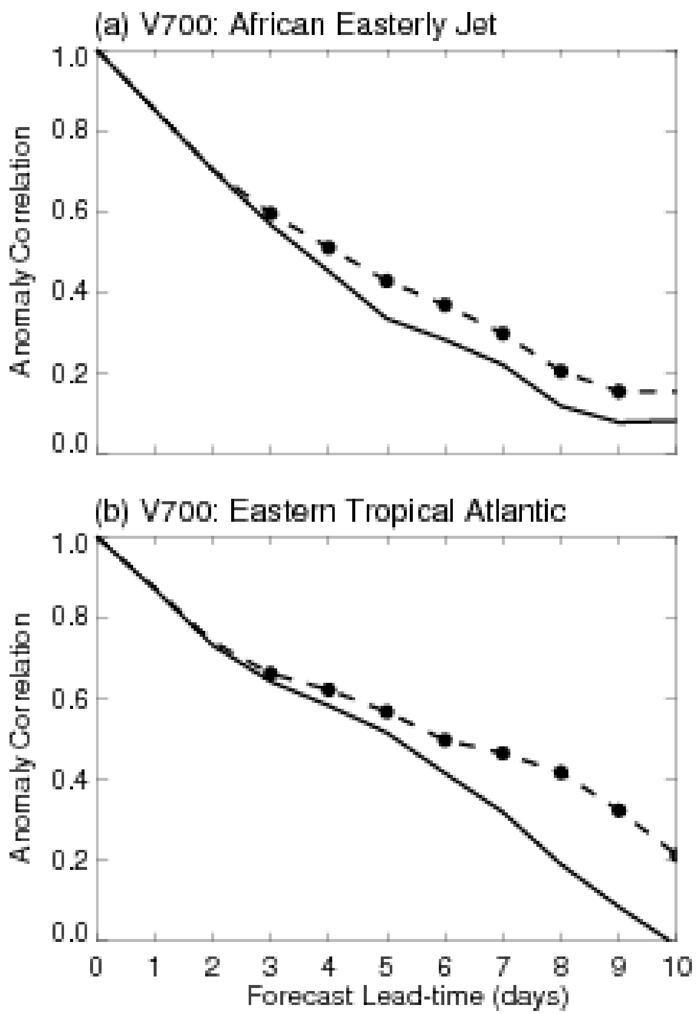
Surface Sensible heat flux differences

20 W m^{-2} ~ 20-30%



Boundary layer height increases >1km

Improved Predictability with improved Aerosol Climatology



New

Old

Improved forecasts of meridional wind variations at 700 hPa for

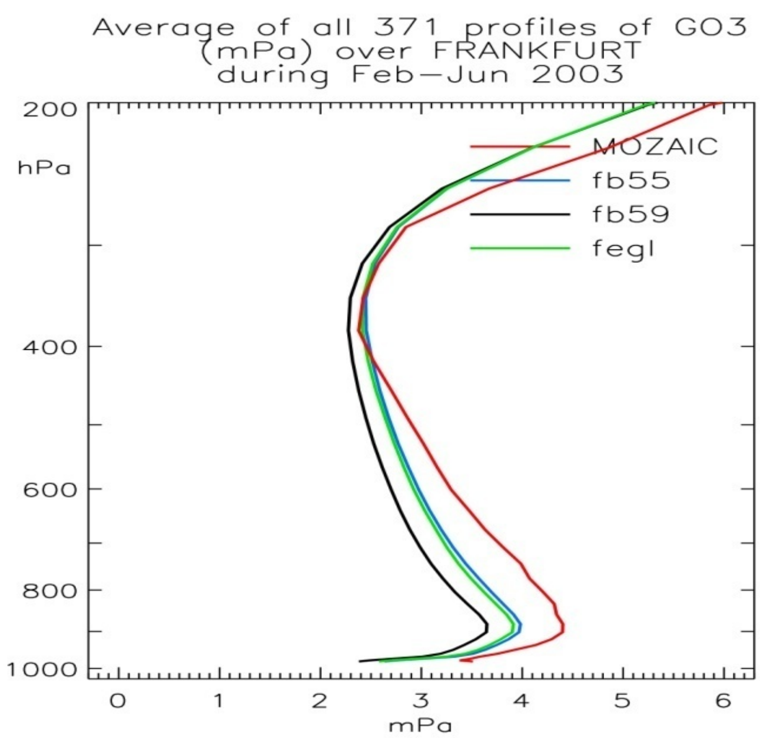
(a) the African easterly jet region and

(b) the eastern tropical Atlantic

Rodwell and Jung (2008), QJRM., **134**, 1479.1497

Benefit of chemical coupling

- **Background NOx levels determine O3 production/loss**
- **Assimilation of NO2 has an impact on ozone field (through chemical feedbacks in the CTM)**
- **Assimilation of NO2 can improve O3 field**



Validation with MOZAIC ozone data

Control (no CO or NO2 assim, only O3 assim)

MOZAIC observation

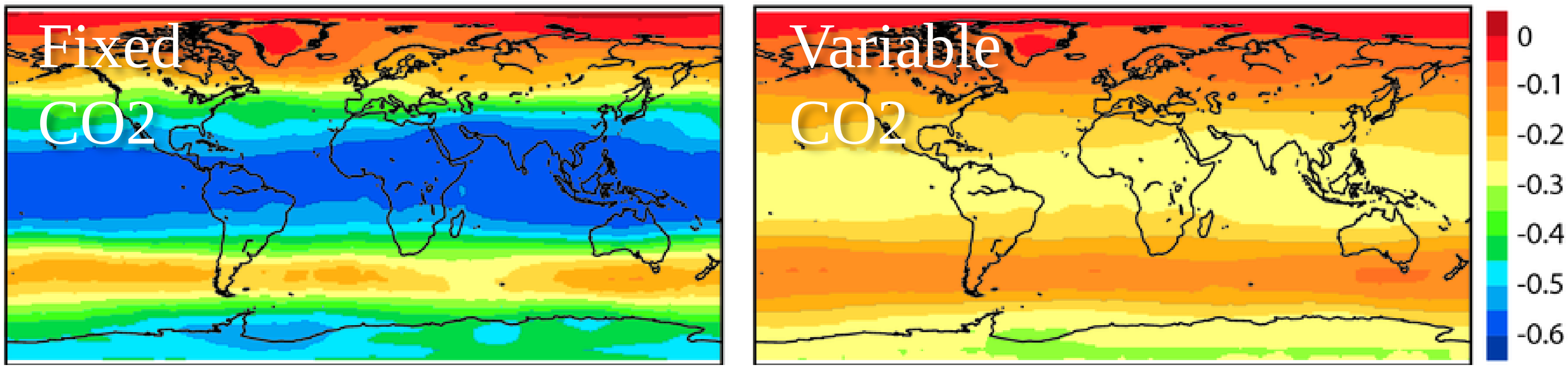
CO & NO2 assim

NO2 assim

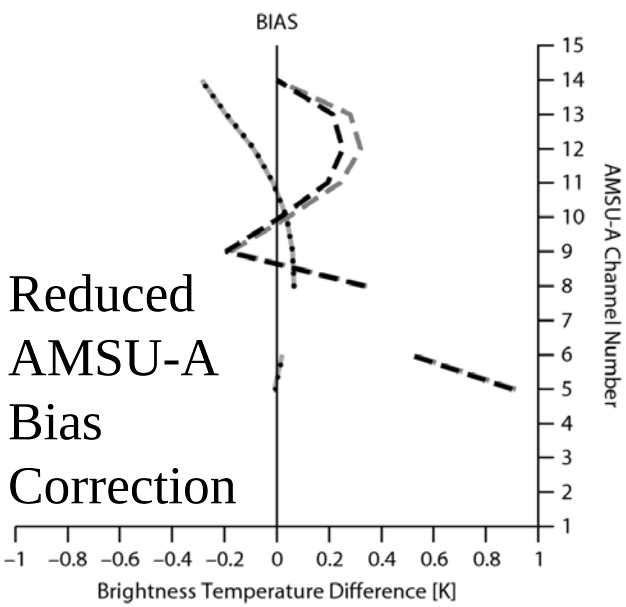
ECMWF

Benefit of trace gases for NWP: VarCO_2 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)



Reduced AMSU-A Bias Correction

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

Use of different approximations instead of fully modelled CO_2 is subject of further study.

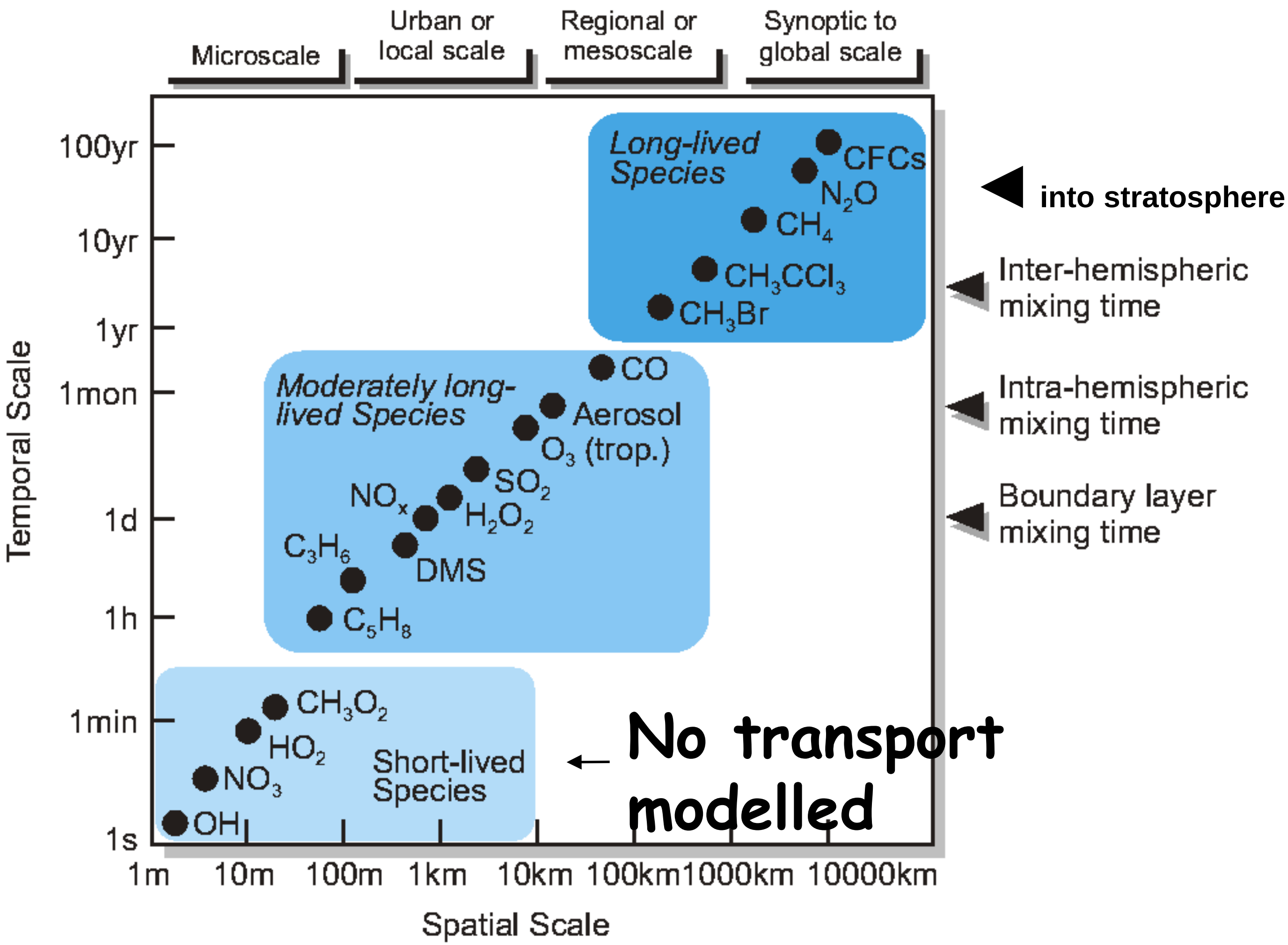
Engelen and Bauer, QJRMS, 2011

CHALLENGES FOR ATM. COMPOSITION DATA ASSIMILATION

Challenges

- **Quality of NWP depends predominantly on initial state**
- **AC modelling depends on initial state (lifetime) and surface fluxes**
- **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**
- **Data availability**
- **More complex and expensive, e.g. atmospheric chemistry, aerosol physics**
- **Concentrations vary over several orders of magnitude**

Chemical Lifetime vs. Spatial Scale



After Seinfeld and Pandis [1998]

Emission Estimates

- Emissions are one of the major uncertainties in modeling
- 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 also used in data assimilation can be used to correct emission estimates using observations and models – in particular for long lived gases such as CO_2 and Methane

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, Methane, 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 …)
- In MACC we use GFAS fire emissions (Kaiser et al. 2012) and MACCity anthropogenic emissions (Granier et al. 2011)
- Biomass burning accounts for ~ 30% of total CO and NO_x emissions, ~10% CH4

Importance of emissions: Hindcast experiments

Huijnen et al. 2012 (ACP)

- *TM5-chem-v3.0 coupled to ECMWF-IFS*
- *'daily' 4 day hindcasts were produced*
- *From 15 July – 31 August 2010*

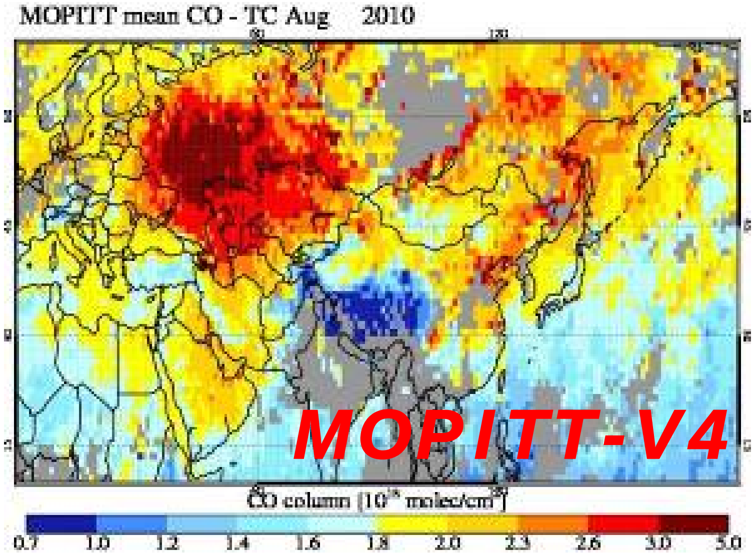
Version	Assimilation	Emissions
Ref	no	GFEDv2 climatology
Assim	CO (IASI), O3 (OMI, MLS), NO2 (OMI)	GFEDv2 climatology
GFAS	no	GFASv1
Assim-GFAS	CO (IASI), O3 (OMI, MLS), NO2 (OMI)	GFASv1

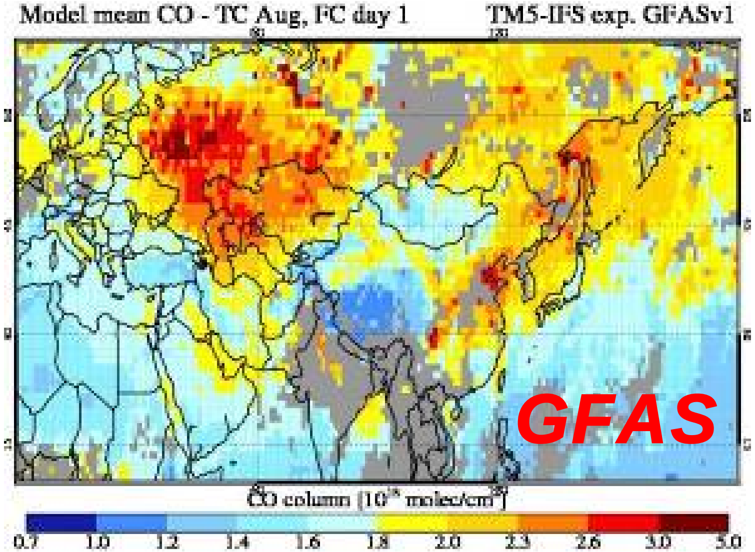
Notes:

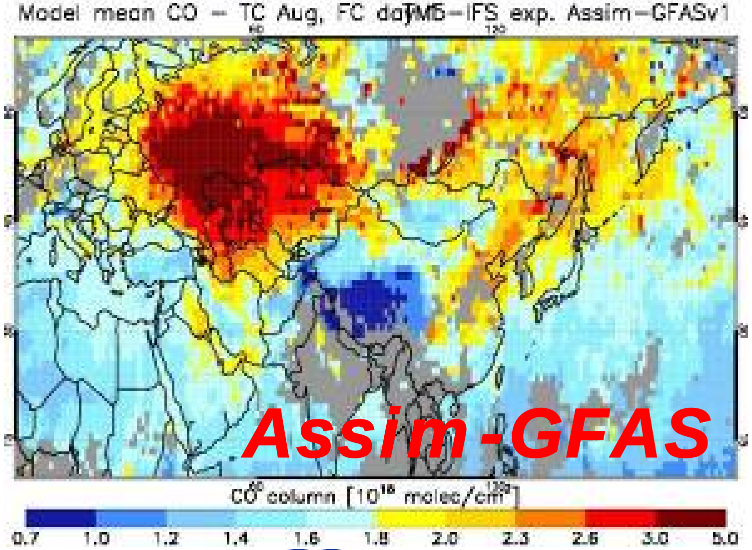
- *One year spin-up (free model run)*
- *RETRO/REAS anthropogenic emissions*
- *In forecasts: persistency of fire emissions*

CO without/with assim vs MOPITT-V4

Huijnen et al. 2012 (ACP)

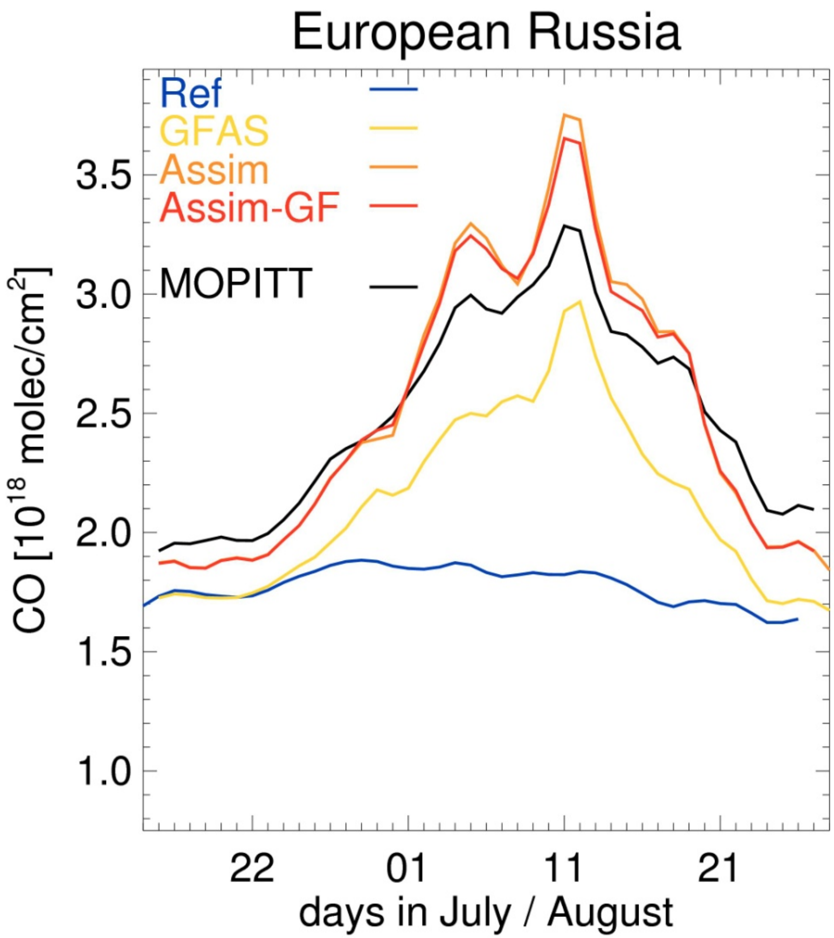






ECMWF

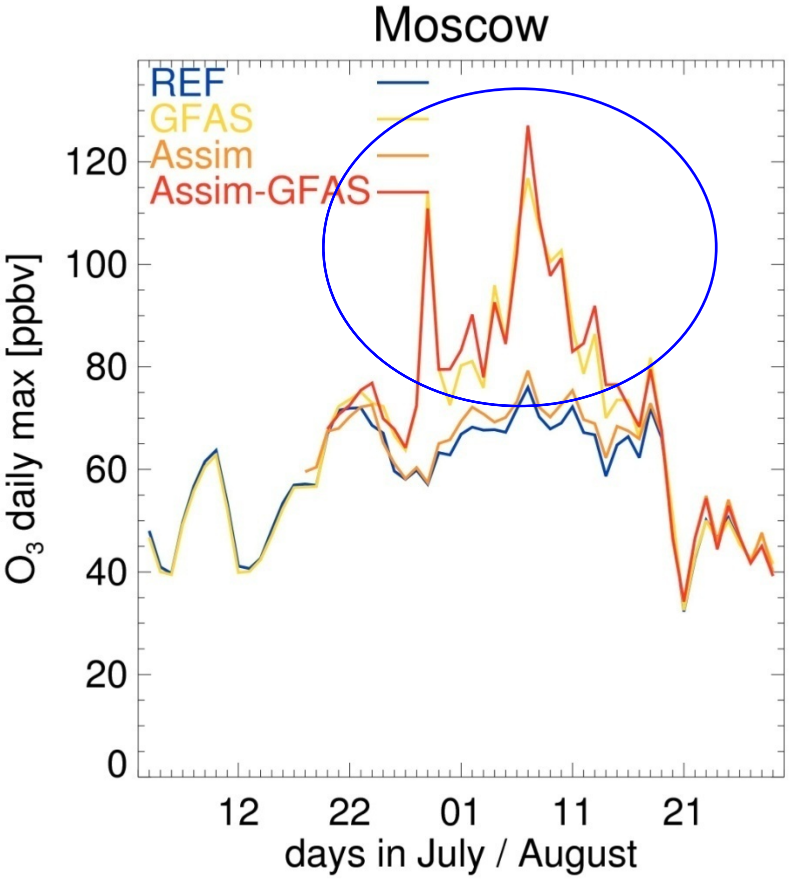
Evolution of CO columns vs MOPITT-V4

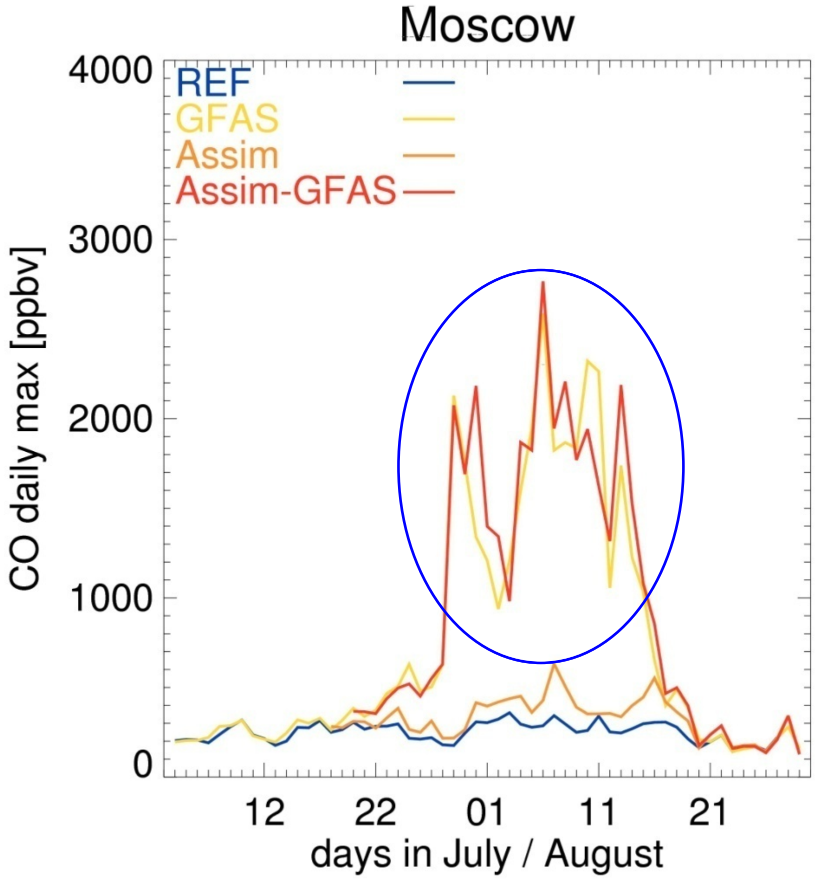


- Assimilation of IASI TCCO leads to improved fit to MOPITT TCCO
- TCCO from Assim and Assim-GFAS very similar

Huijnen et al. 2012 (ACP)

Daily maximum surface O_3 and CO concentrations

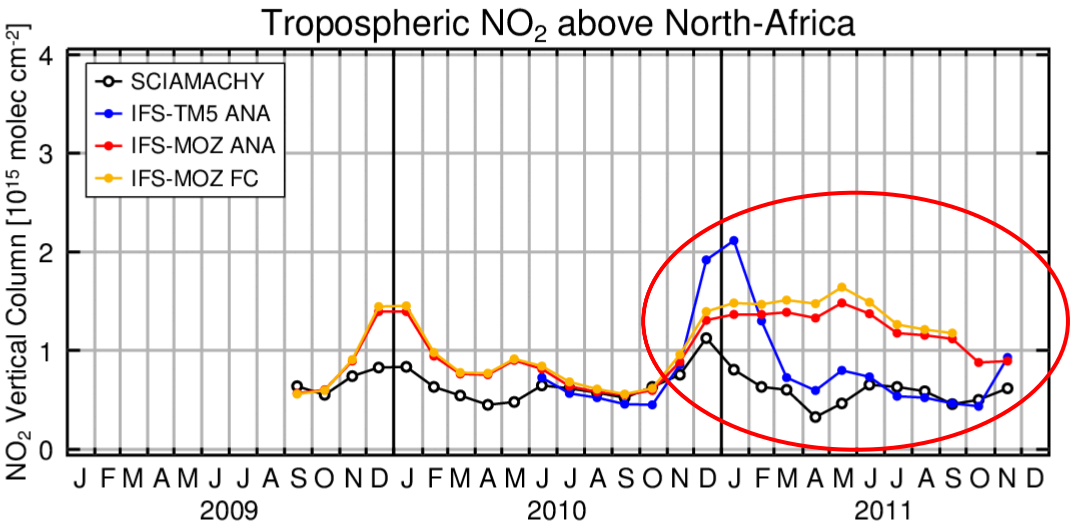


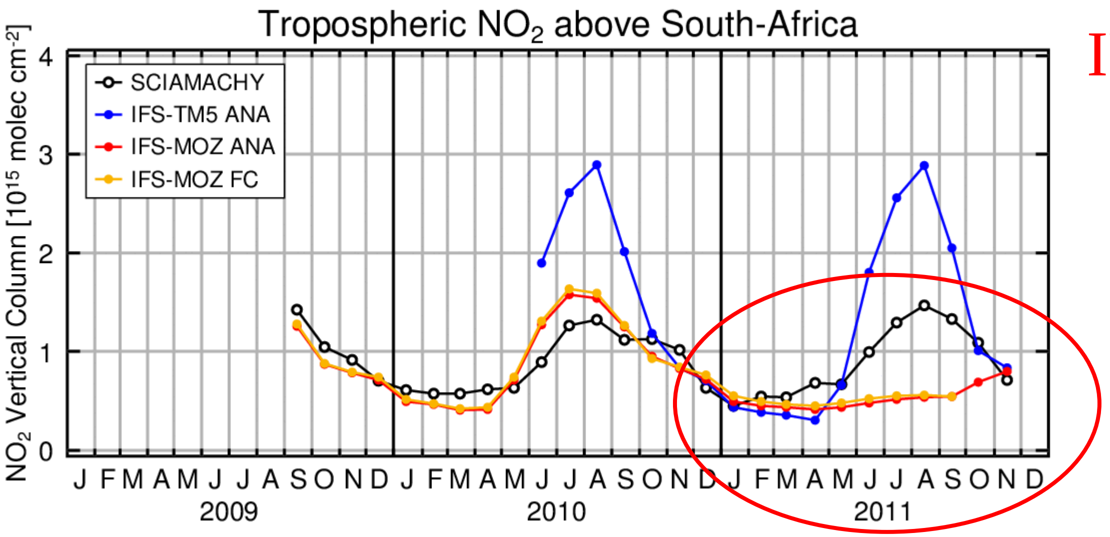


GFAS emissions are needed to get peak in surface concentrations

Huijnen et al. 2012 (ACP)

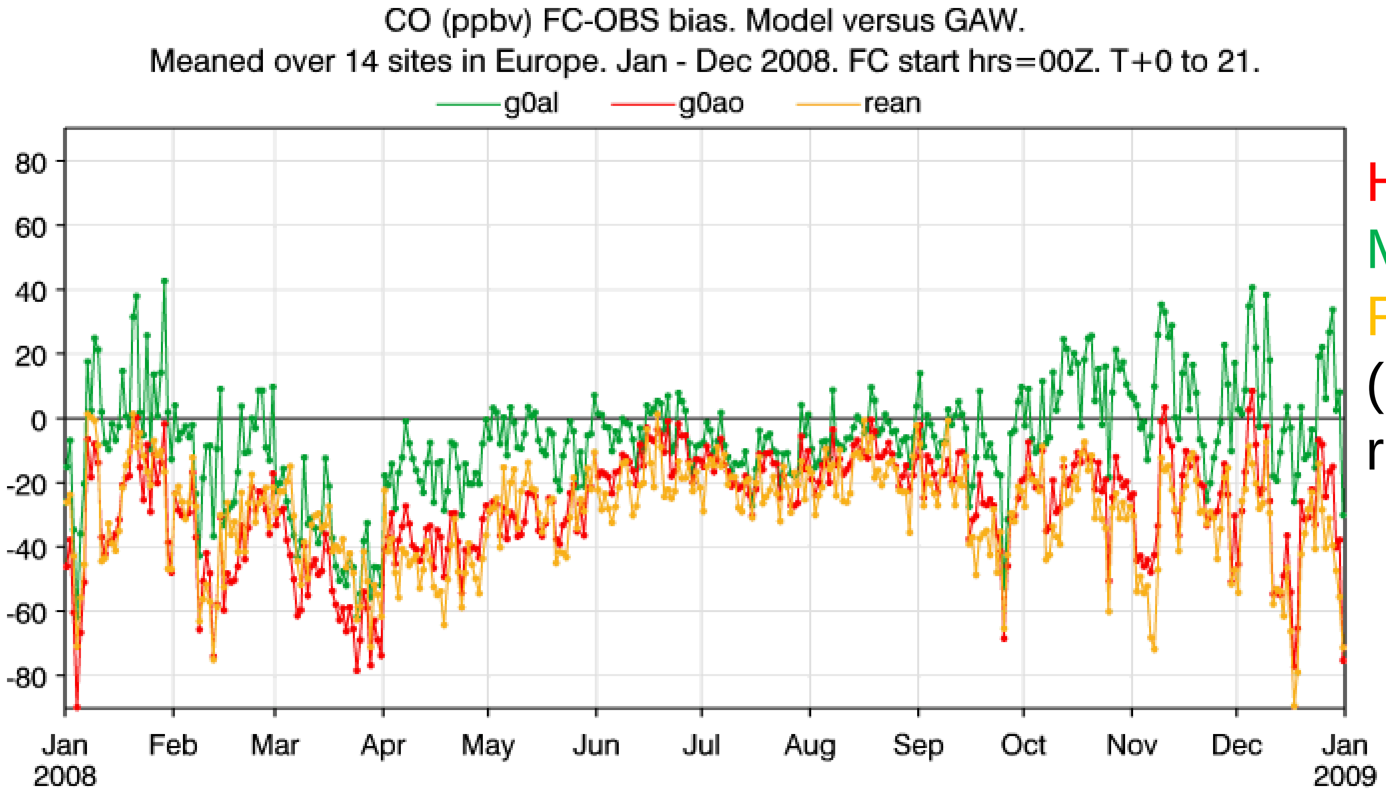
Importance of fire emissions on tropospheric NO2





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

Impact of anthropogenic emissions: CO Bias GAW Europa timeseries



HTAP emissions
MACCity emissions
Reanalysis
(GFAS used in all runs)

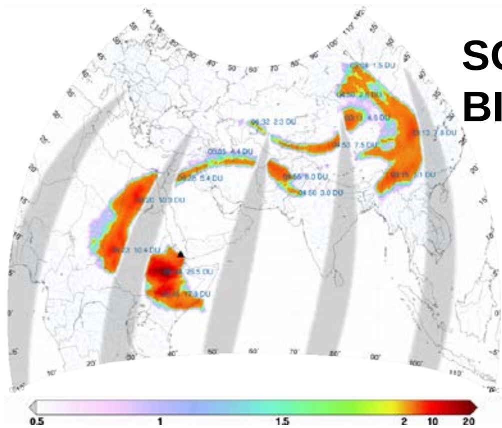
Choice of emissions data set has large impact on surface concentrations

J. Flemming

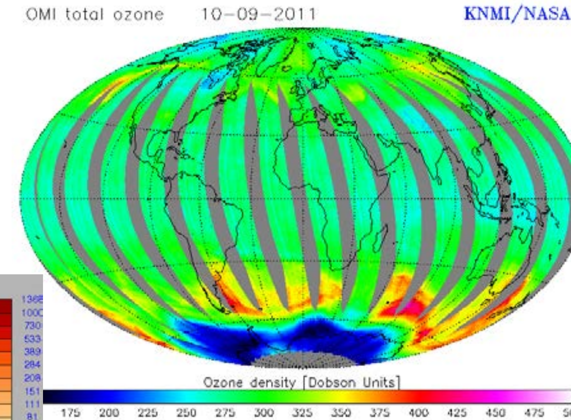
OBSERVATIONS OF ATMOSPHERIC COMPOSITION

Satellite observations

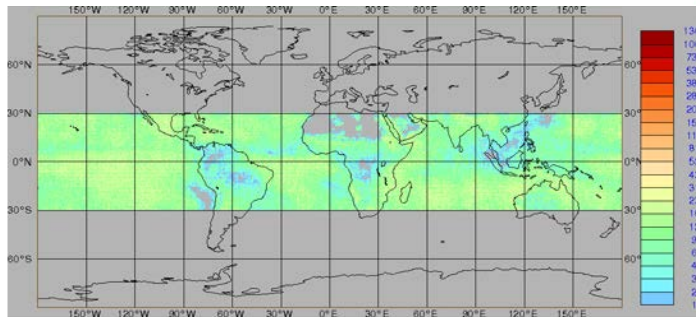
SO_2, GOME-2, SACS, BIRA/DLR/EUMETSAT



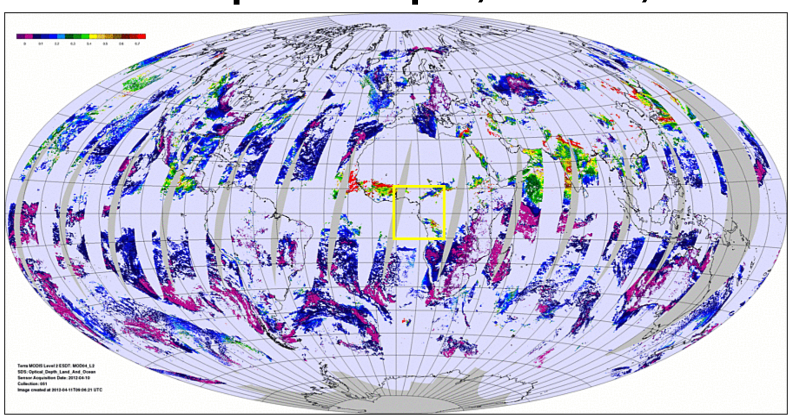
O_3, OMI, KNMI/NASA



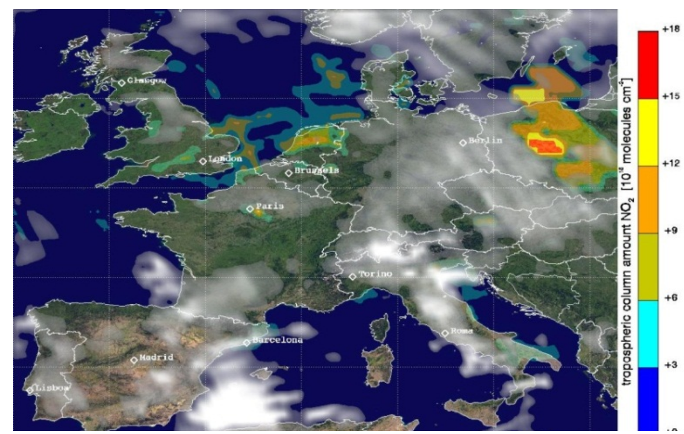
CH_4, IASI, LMD



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 only. Infrared/microwave are now adding more and more to this spectrum of observations (MOPITT, AIRS, IASI, MLS, MIPAS …)

Issues with Observations

- **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**
  - **We use retrievals for AC: Averaging kernels important**
- **AC in-situ observations**
  - **Sparse (in particular profiles)**
  - **Limited or unknown spatial representativeness**

Importance of height resolved observations

Impact of a single observation in 3D-Var
(for model variable at a gridpoint)

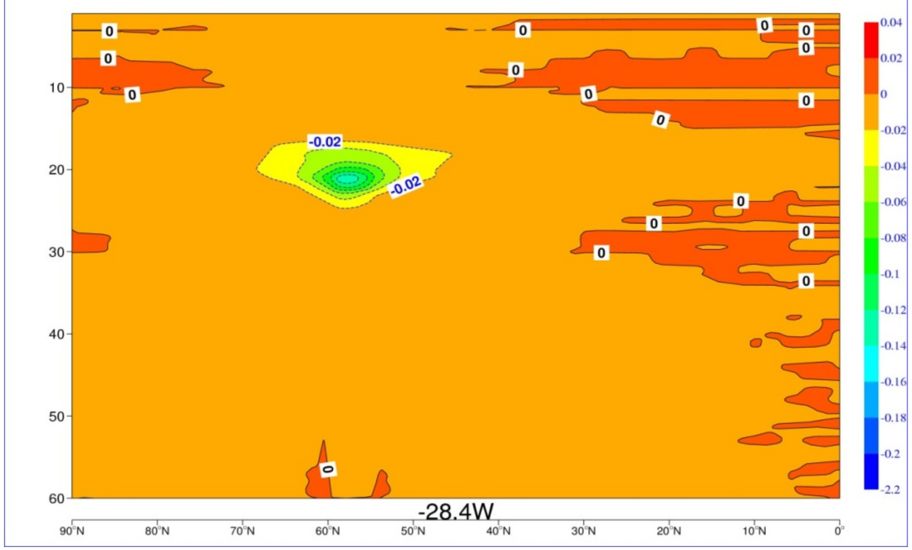
$$x_a - x_b = \frac{y - x_b}{\sigma_o^2 + \sigma_b^2} B$$

- x_a: analysis value
- x_b: background value
- y: observation
- σ_o^2: observation variance
- σ_b^2: background covariance
- B: column of background error covariance matrix

- Analysis increment is proportional to a column of B-matrix
- B-matrix determines how increment is spread out from a single observation to neighbouring gridpoints/ levels

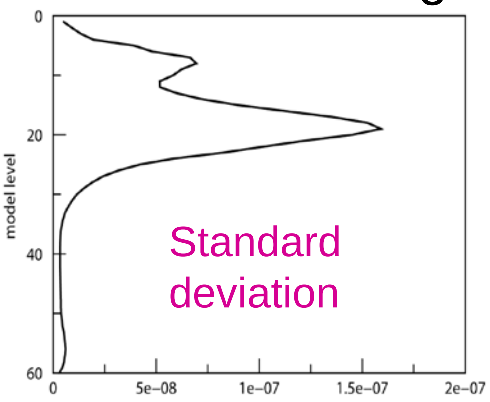
Increment from a single TCO3 observation

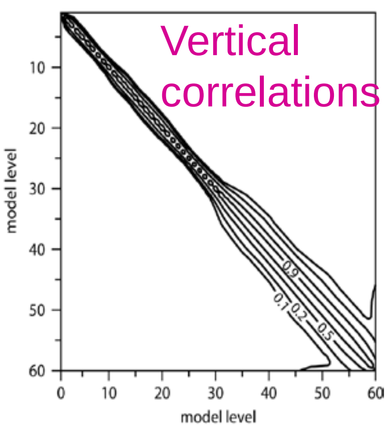
Increment created by a single O3 obs

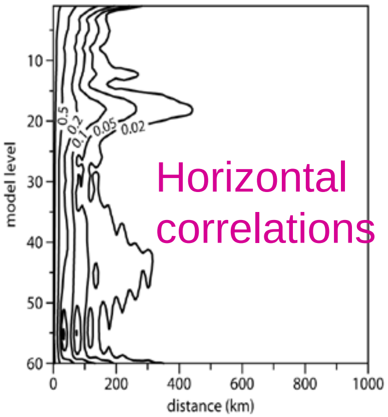


Ozone observation of 247 DU, 66 DU lower than background

Ozone background errors

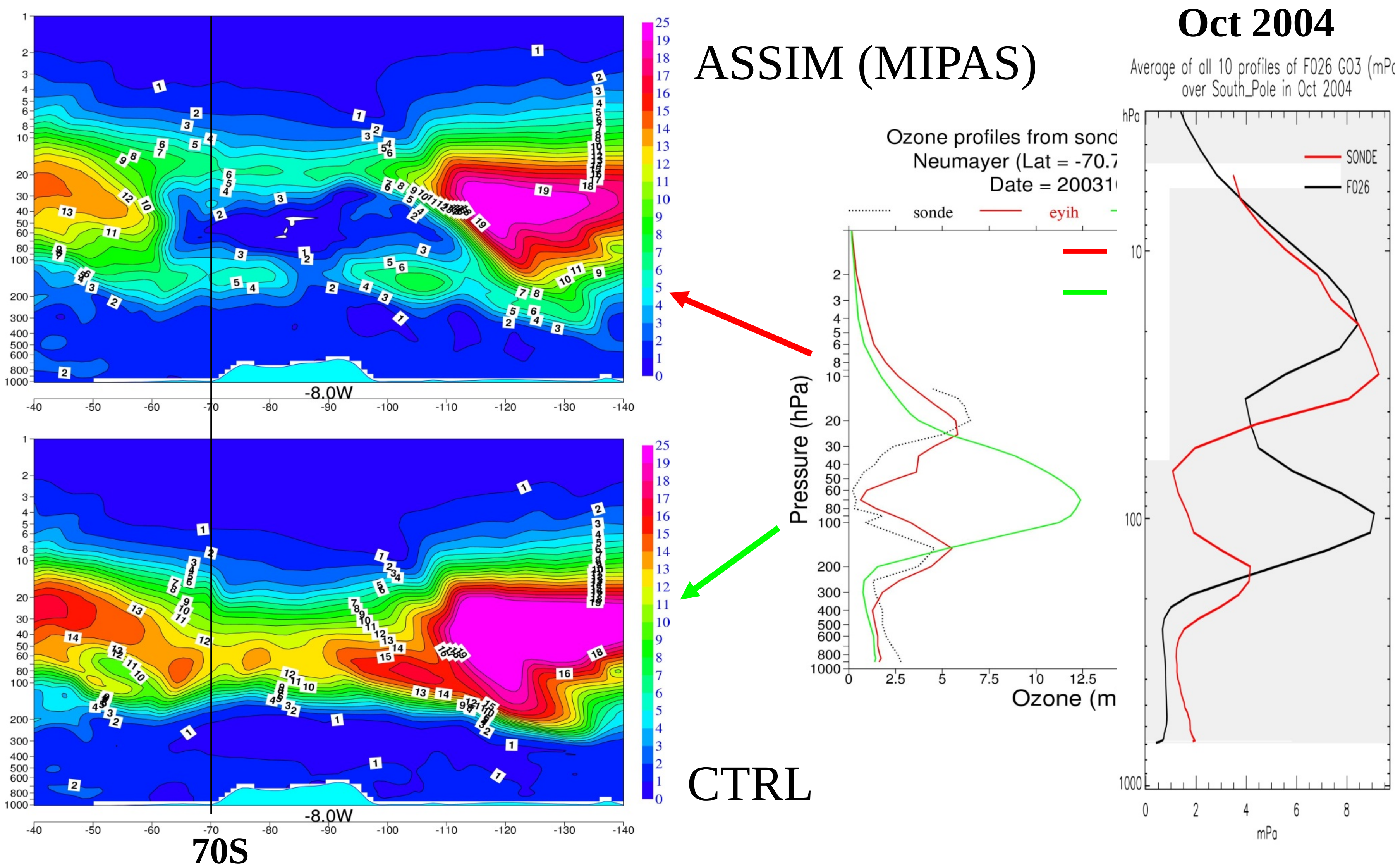






Profile data are important to obtain a good vertical analysis profiles

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



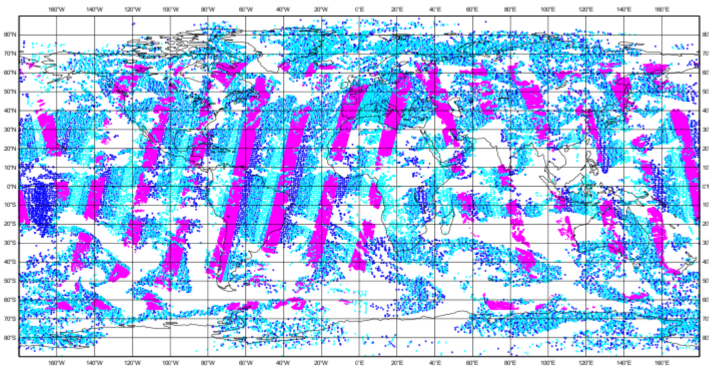
REACTIVE GASES DATA ASSIMILATION

Setup for the reactive gases assimilation

- **IFS species: O3, CO, NO2, SO2, HCHO**
- **More species available from CTM output (and in C-IFS)**
- **Coupled system or C-IFS**
- **Background errors calculated with:**
  - **NMC method (CO, NOx, HCHO)**
  - **Analysis ensemble method (O3)**
  - **Prescribed profile (SO2)**
- **Difficulties assimilating species with short lifetimes (e.g. NO2): NOx as control variable and NO2-NOx interconversion operator**
- **Variational bias correction (Hans Hersbach's lecture) used for reactive gases**
- **Chemistry included in outer loop (ifstraj) not in minimisation; adjoint of transport only**

Reactive gases data usage in MACC NRT system: 20130801, 12z

CO

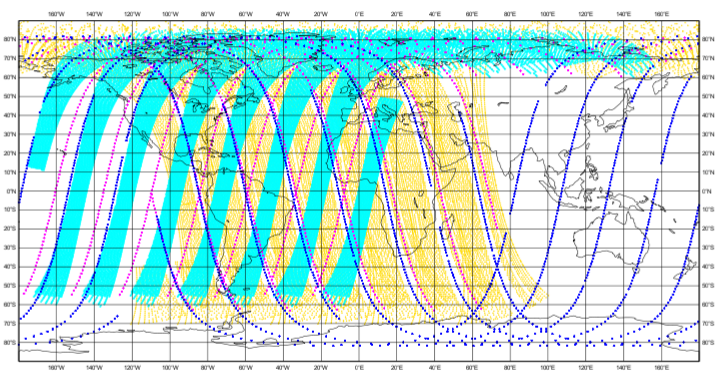


IASI Metop-A

IASI Metop-B

MOPITT TERRA

O3



GOME-2 Metop-A

OMI AURA

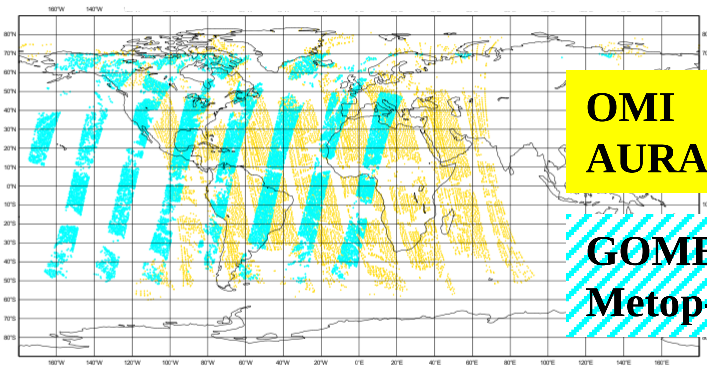
MLS AURA

SBUV/2 NOAA-16 NOAA-19

assimilated

monitored

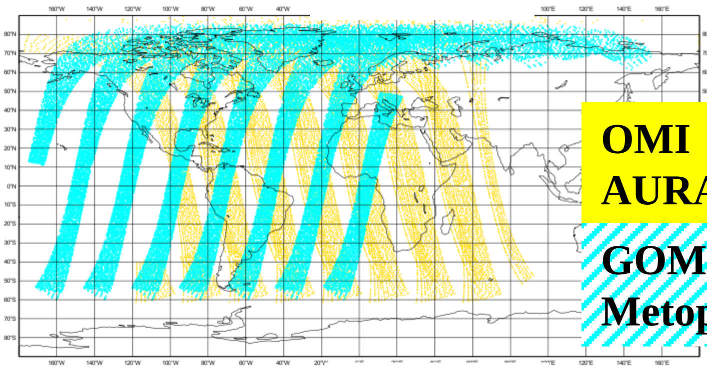
Tropospheric NO2



OMI AURA

GOME-2 Metop-A

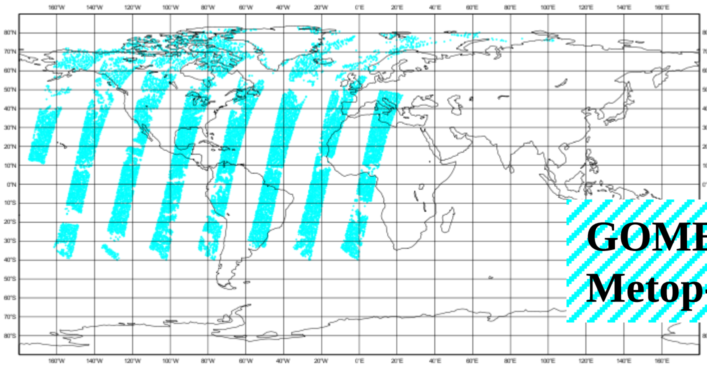
SO2



OMI AURA

GOME-2 Metop-A

HCHO

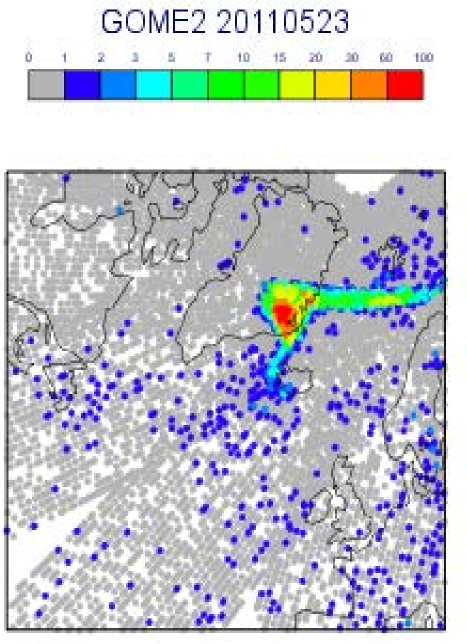


GOME-2 Metop-A

Use of GOME-2 data for SO2 plume forecasts for 2011 Grímsvötn and 2010 Eyjafjallajökull eruptions

Two ways to forecast SO2 plumes:

- **Estimate source strength and injection height and simulate transport with model ("CTM" -style)**
- **Assimilate initial SO2 fields (initial conditions) and model transport ("NWP"-style)**



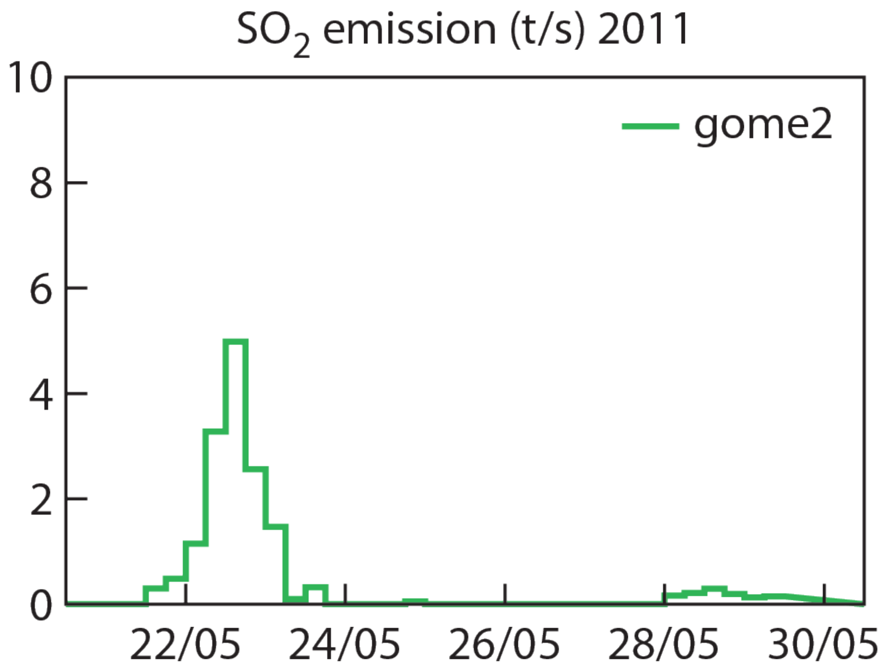
- Use GOME-2 data to estimate volcanic SO2 emissions and injection heights
- Assimilate GOME-2 SO2 data to provide initial conditions for SO2 forecasts
- Both methods allow NRT SO2 forecasts for volcanic eruptions

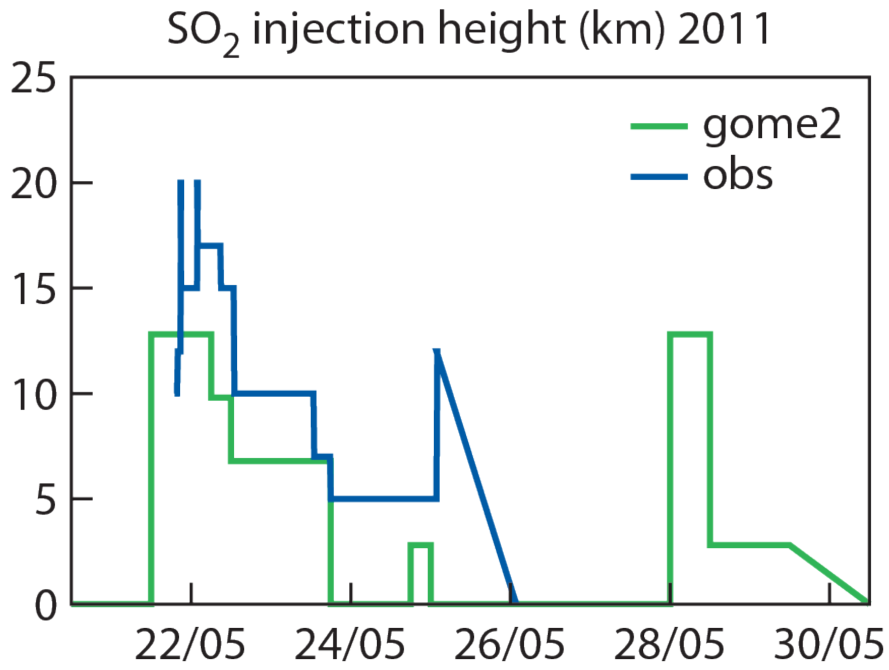
Flemming and Inness (JGR, 2013)

GOME-2 data provided by DLR

Estimated plume strength and height information from satellite observations

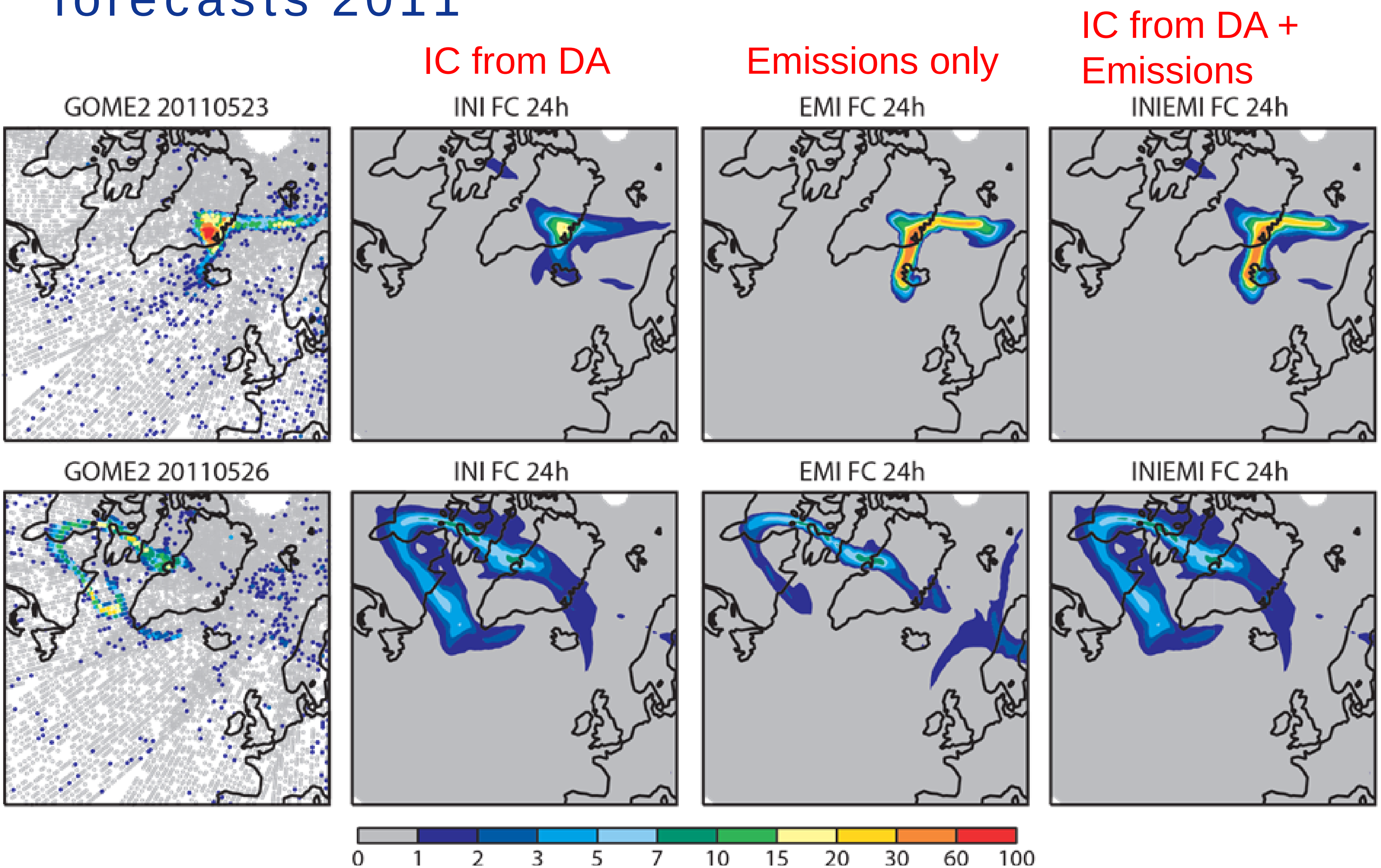
1. **Release test tracer (E_{test}=1 t/s) at different levels - find best match in position**
2. **Scale emissions of test tracer and observations to get emission estimate**





Plume top height obs from a synoptic radar at Keflavik airport (Petersen et al. 2012)

Assimilation of GOME-2 SO2 and 24h SO2 forecasts 2011



The initialization with GOME-2 SO2 analyses (INI and INIEMI) improved in particular the forecast of the Grímsvötn plume after the end of the eruption.

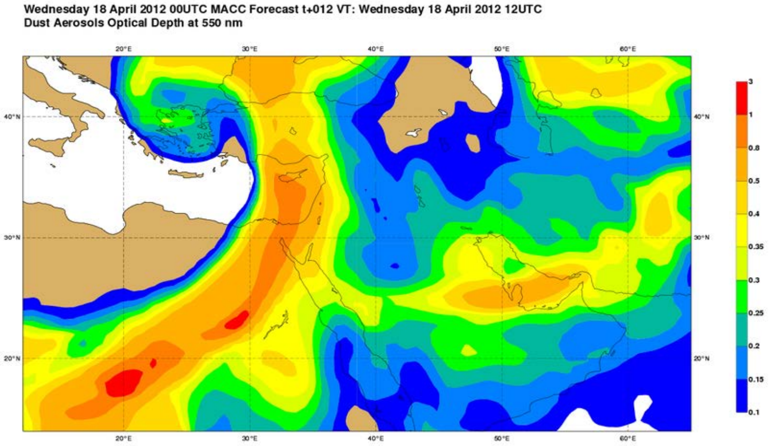
More in Flemming and Inness (2013, JGR)

AEROSOL DATA ASSIMILATION

4D-Var assimilation system for aerosols

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**



ECMWF

The aerosol prediction system: Forward model

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

fine mode
coarse mode

Physical processes include:

• emission sources (some 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)

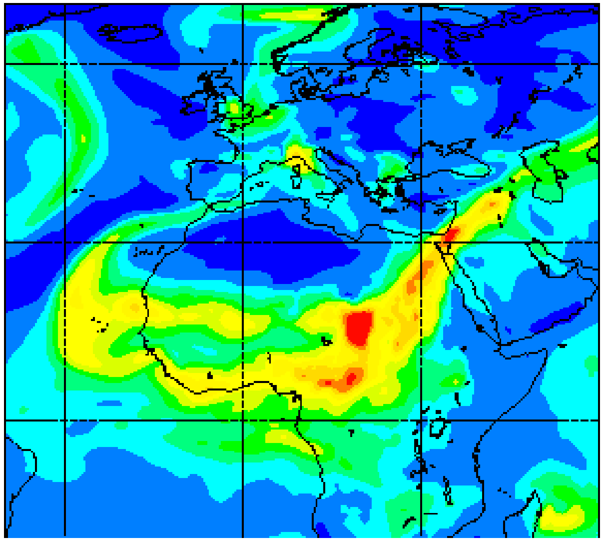
The aerosol prediction system: Analysis

- **Assimilated observations are the 550nm MODIS Aerosol Optical Depths (AODs) over land and ocean, and the fine mode AODs over ocean.**
- **Control variable is formulated in terms of the total aerosol mixing ratio.**
- **To come *dual mode control variable*: aerosol control variables are the fine mode (<1 μm diameter) and coarse mode aerosol mixing ratio. Analysis increments are repartitioned into the species according to their fractional contribution to the fine/coarse mode mixing ratio.**
- **Background error statistics were computed using forecasts errors as in the NMC method (48h-24h forecast differences).**
- **Observation errors are prescribed fixed values.**
- **Variational bias corrections are applied to both total and fine mode AOD.**
- **Improvements of dual mode control variable are especially seen in fine mode AOD**

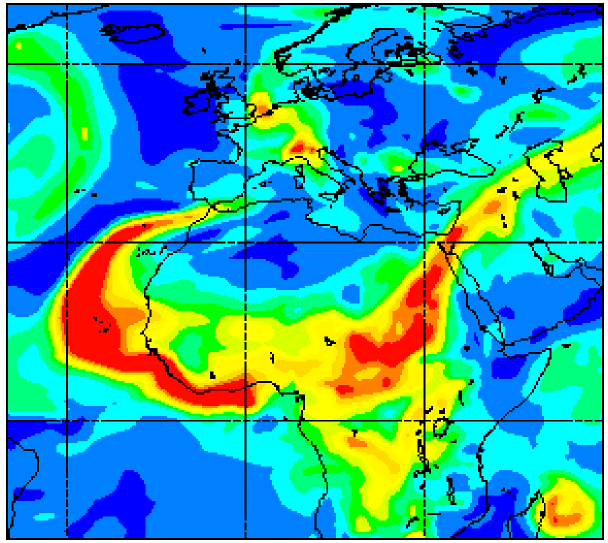
Angela Benedetti

Saharan dust outbreak: 6 March 2004

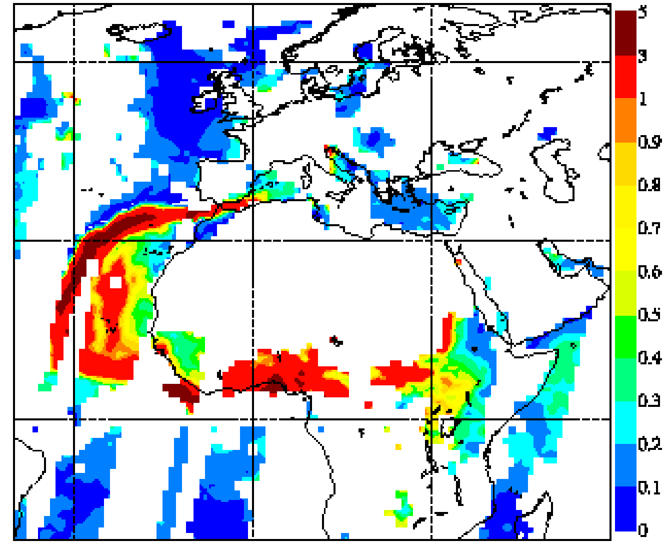
Model simulation



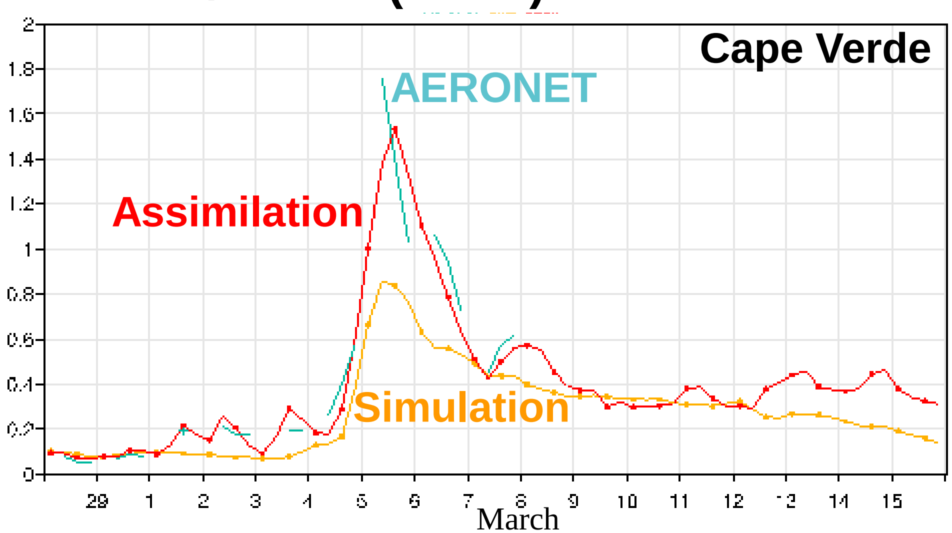
Assimilation

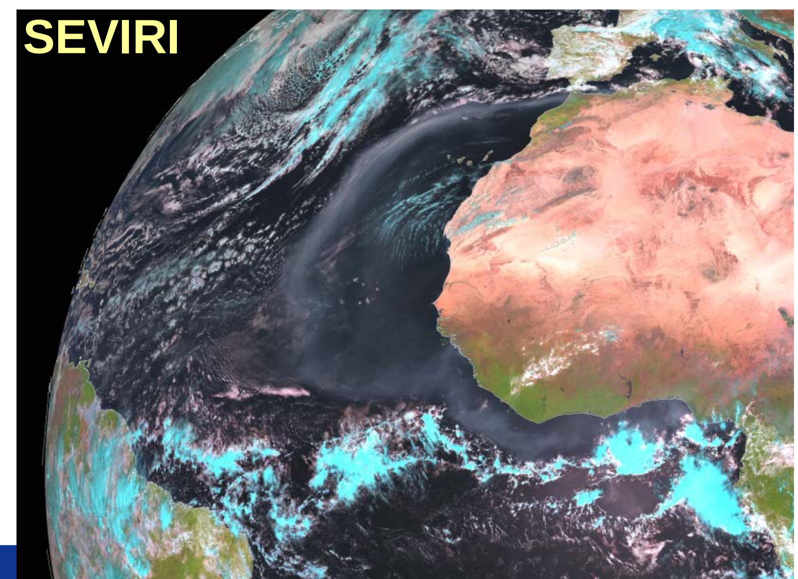


MODIS

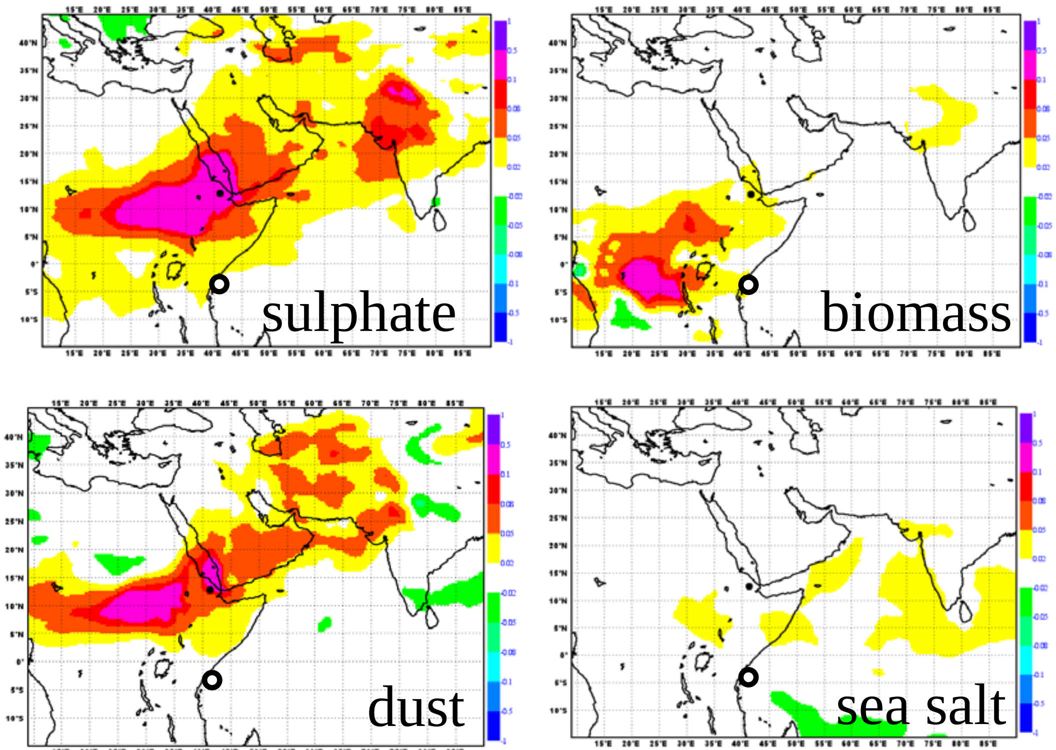


Aerosol optical depth at 550nm (upper) and 670/675nm (lower)



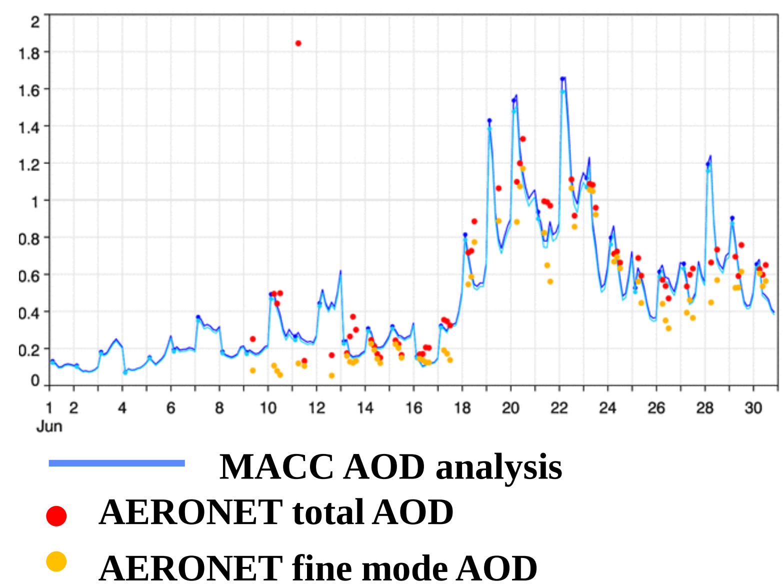


Example for wrong aerosol attribution



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

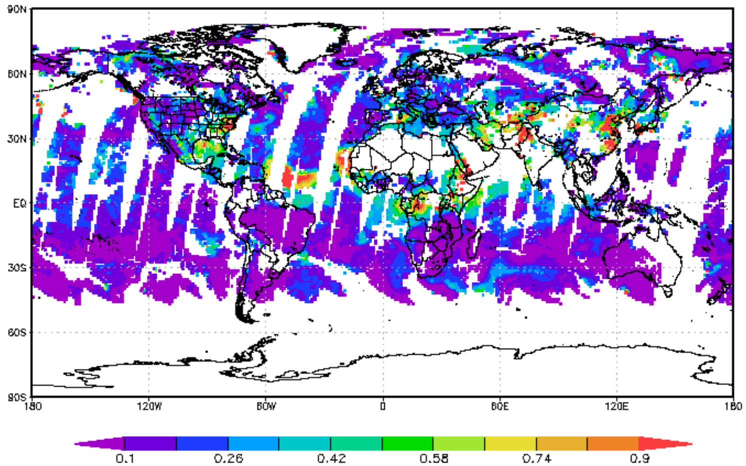
ICIPE-Mbita - AERONET

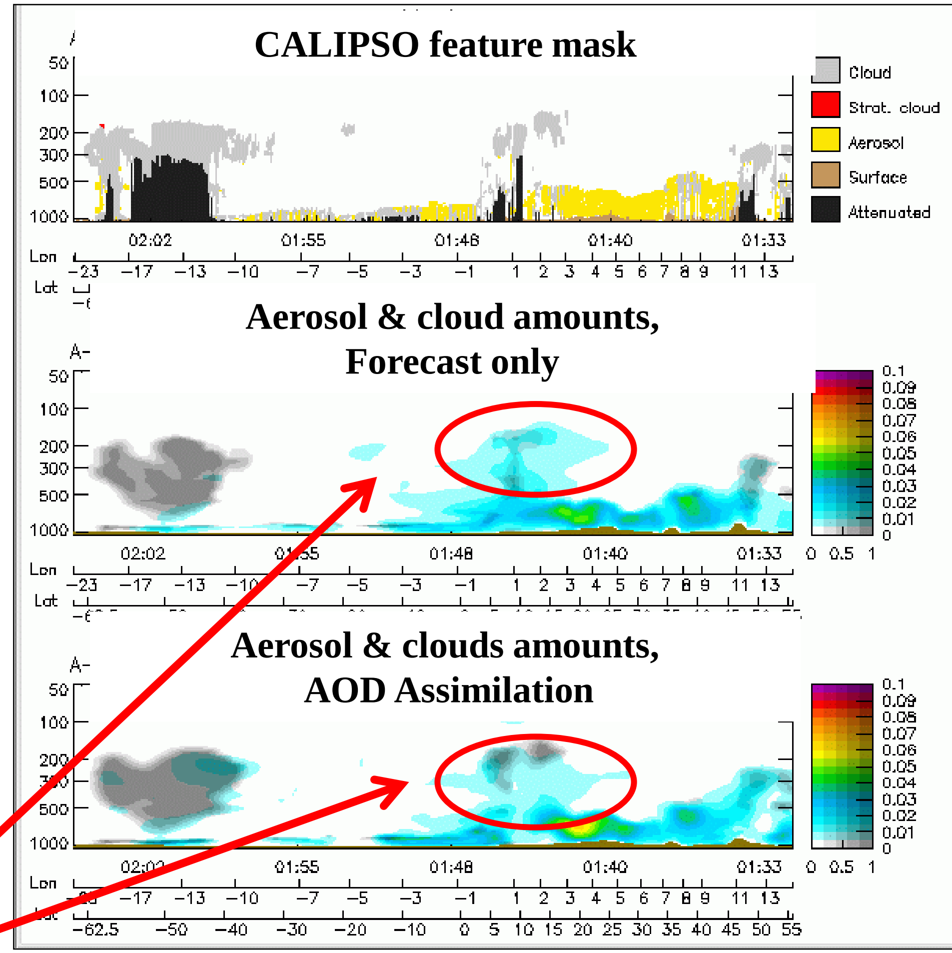


The MACC aerosol model did not contain stratospheric aerosol at this time, so the observed AOD was wrongly attributed to the available aerosol types.

Why we need profiling data for aerosol assimilation

MODIS Aerosol Optical Depth





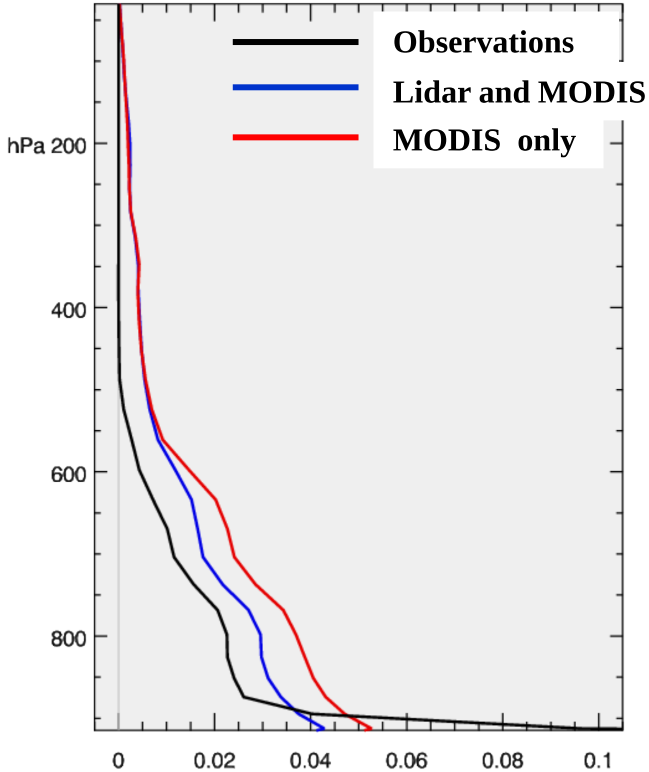
- **AOD is a column-integrated quantity**
- **Assimilation of AOD does not modify the vertical profile**
- **Profile data are needed (lidar)**

Graphics by Luke Jones

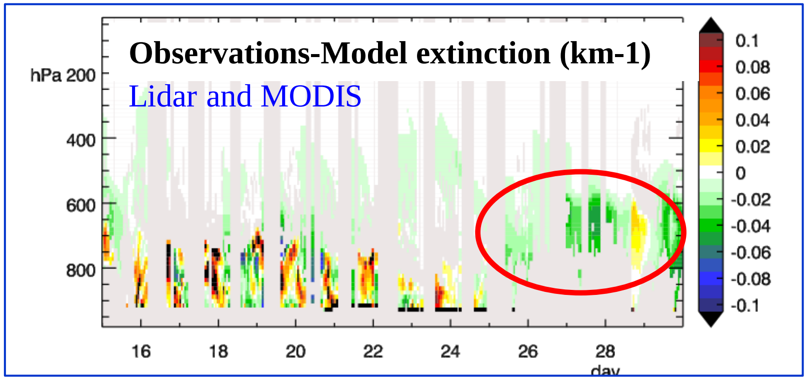
ECMWF

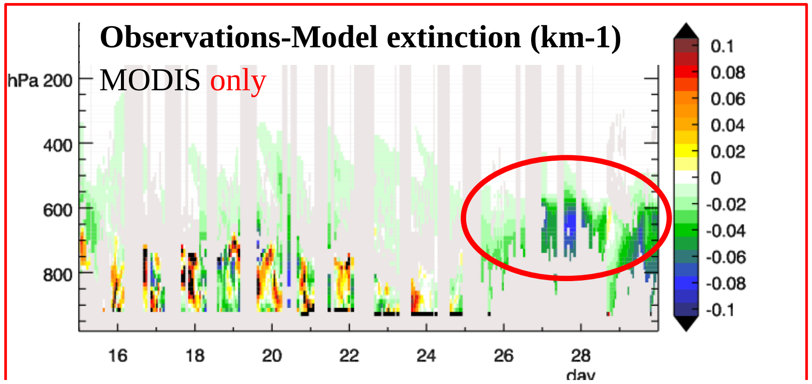
Towards lidar assimilation: Impact of Calipso on vertical profiles

- NRT CALIPSO level 1.5 product available since mid-2011
- Mean Attenuated aerosol backscatter at 532 nm (cloud cleared)
- Aimed at operational NWP centres (ECMWF, US Naval Research Lab, JMA,…)
- Developed through close collaboration with NASA LaRC CALIPSOTeam
- Lidar observation operator in place and performing well
- Clipso data have positive impact on the aerosol extinction profile (in initial tests)



Monthly averaged extinction (km^{-1}) at 532nm at Sede Boker (453 profiles)





(*) Lidar data are courtesy of Arnon Karnieli. Special thanks to Simone Lolli, Judd Welton and the MPLNET team.

Concluding remarks

- Atmospheric composition (AC) and weather interact
- IFS has been extended to include fields of atmospheric composition: Reactive gases, greenhouse gases, aerosols
- Modelling of AC needs to include many species with concentrations varying over several orders of magnitude
- AC forecast benefit from realistic initial conditions (**data assimilation**) but likewise from improved emissions
- Extra challenges for DA of atmospheric composition compared to NWP - but also extra benefits through chemical coupling and impact on NWP

- MACC system produces useful AC forecast and analyses, freely available

More information about the environmental monitoring activities at ECMWF and how to access the data can be found on:

http://www.gmes-atmosphere.eu

For questions contact:

info@gmes-atmosphere.eu

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