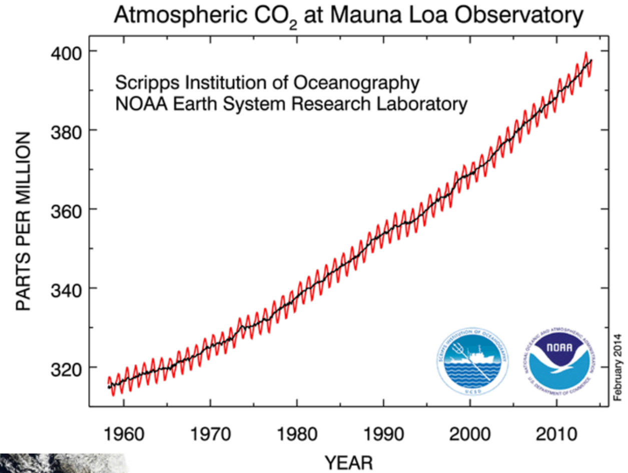
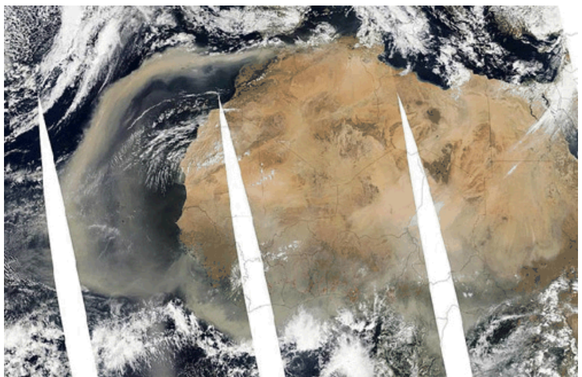
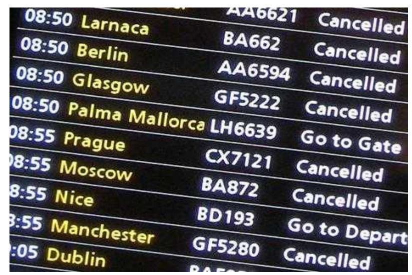
Atmospheric composition







Data Assimilation of Atmospheric Composition

Antje Inness

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

Outline

1. Introduction
2. Potential benefit for NWP
3. Challenges for atmospheric composition DA
4. Observations of atmospheric composition
5. Aerosol assimilation
6. Concluding remarks

1. Introduction

- Environmental and health concern
- Important to provide air quality forecasts
- Expertise in data assimilation and atmospheric modelling
- Not principally different from meteorological DA but several new challenges
- Interaction of atmospheric composition (AC) and NWP
  - Feedback on dynamics via radiation scheme
  - Precipitation and clouds
  - Satellite data observations influenced by aerosols (and trace gases)
  - Hydrocarbon (Methane) oxidation is water vapour source
  - Assimilation of AC data can have impact on wind field

Composition-IFS (C-IFS)

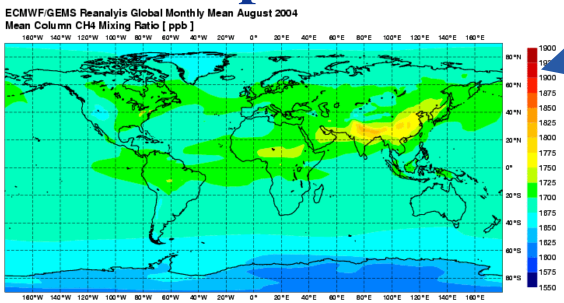
- Over the last decade IFS has been extended with modules for atmospheric composition (aerosols, reactive gases, greenhouse gases)
- GEMS -> MACC -> CAMS (Copernicus Atmosphere Monitoring Service) projects
- At first a "Coupled System", now composition fully integrated into IFS
- Data assimilation of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

MACC/ CAMS Service Provision

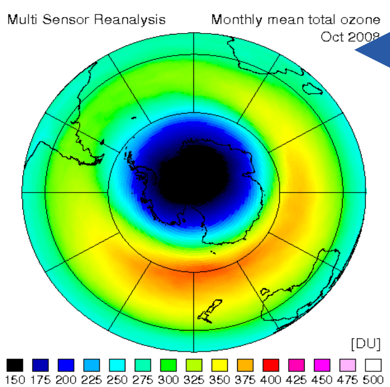
Retrospective

Reanalysis

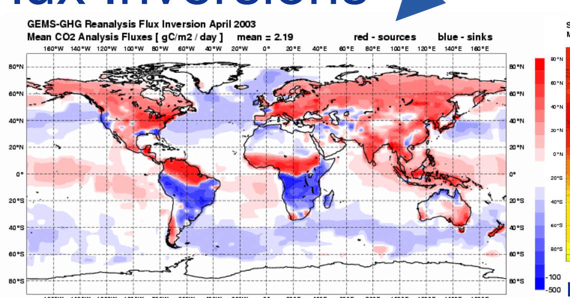
2003-2012



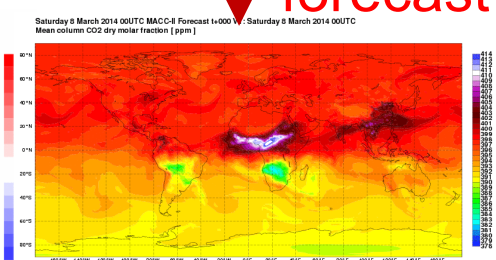
Ozone records



Flux Inversions

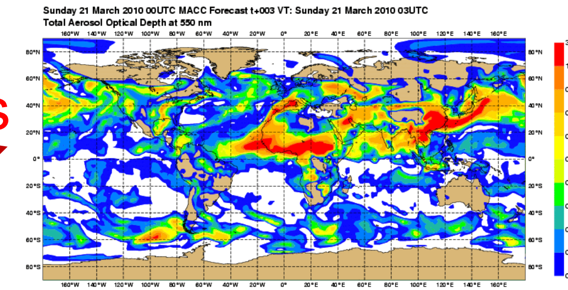


CO_2 forecast

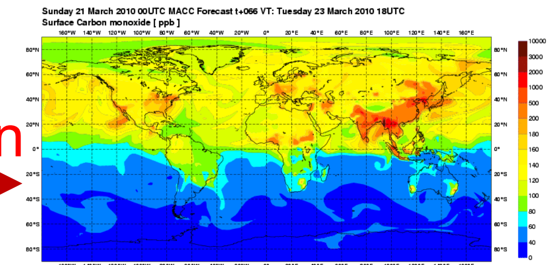


Daily (NRT)

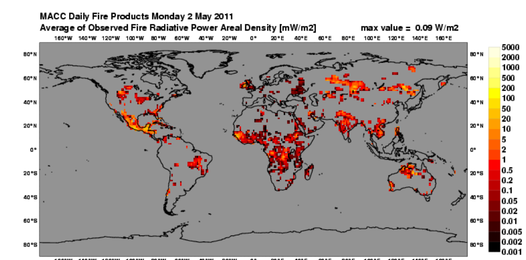
Aerosols



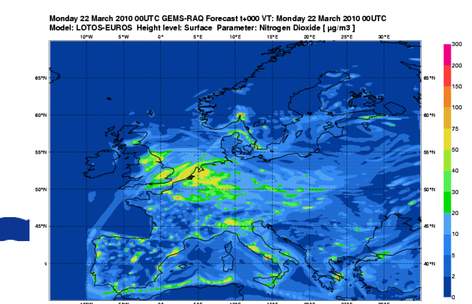
Global Pollution



Fires



Air quality



www.copernicus-atmosphere.eu

MACC 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

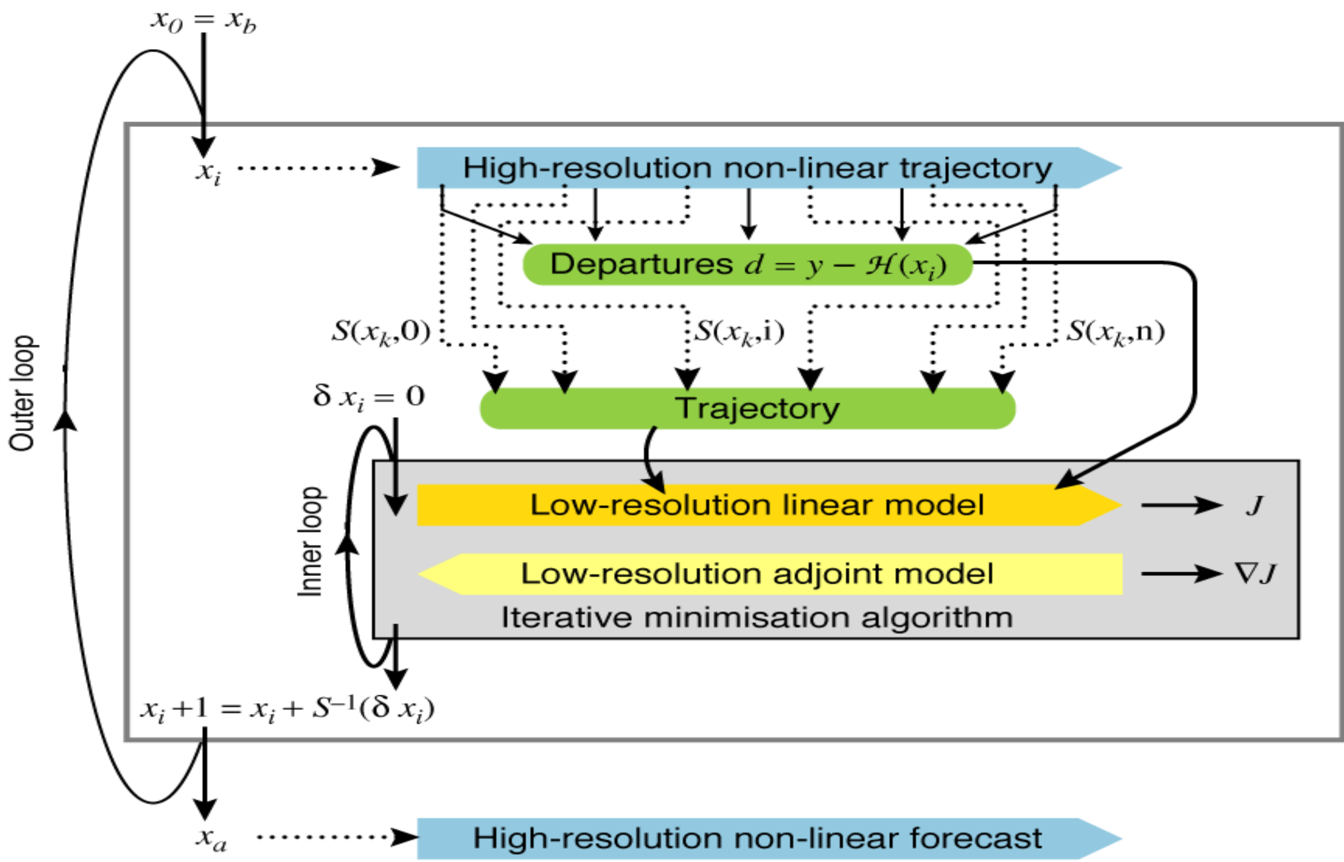
Aerosol model with 12 bins (no TL or AD)

GHG fields

Observations

- Observation operators
- Varbc
- Background error statistics

ECMWF MACC 4D-VAR Data Assimilation Scheme
Assimilation of Reactive Gases



transport + chemistry + aerosol model

advection only

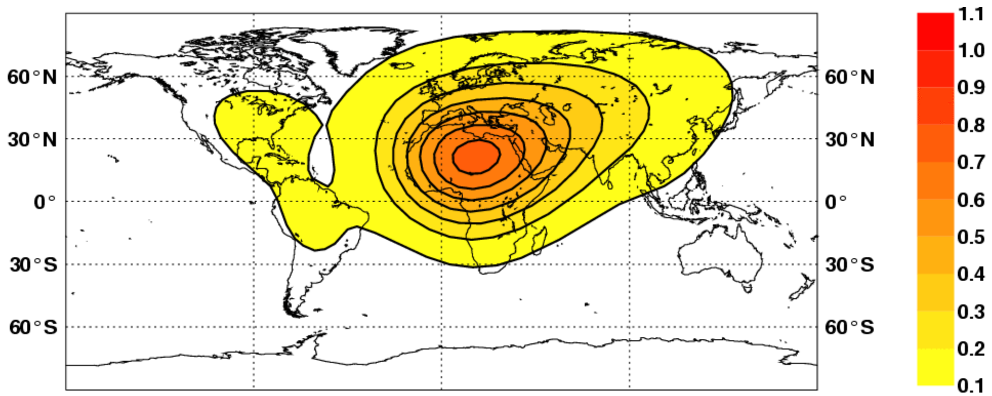
transport + chemistry + aerosol model

ECMWF

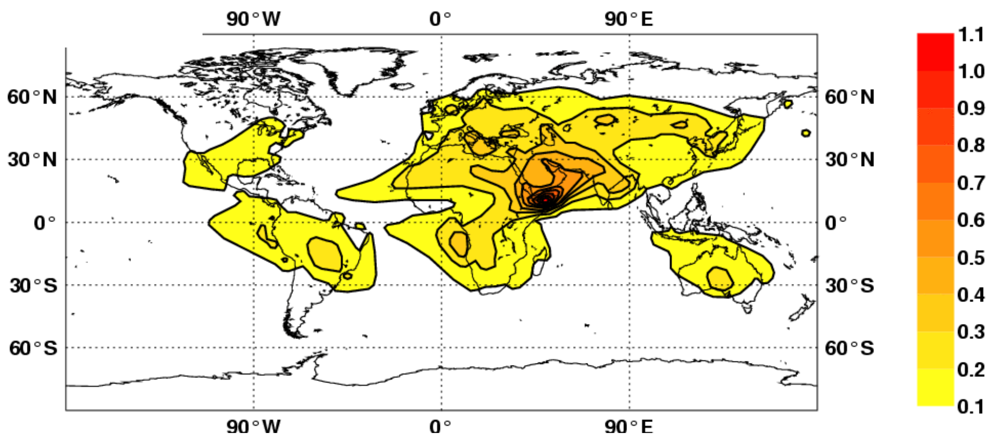
2. Potential benefit for NWP

- Interactive aerosols: Feedback on dynamics via radiation scheme:
  Tegen AER climatology used in radiation scheme (work in progress)
- Use of O_3 (& other fields) in the radiation scheme:
  MACC climatologies used
- RTTOV observation operator: Use of MACC O_3, CO_2 analysis fields to improve the use of radiances sensitive to O_3, CO_2:
  O_3 is used, but climatologies for other tracers (e.g. fixed CO_2 value)
- Dynamical coupling with wind/ T through TL and AD: turned off
- Multivariate JB: Correlations between tracers and dynamical variables, e.g. O_3 and vorticity; correlations between chemical species: univariate

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

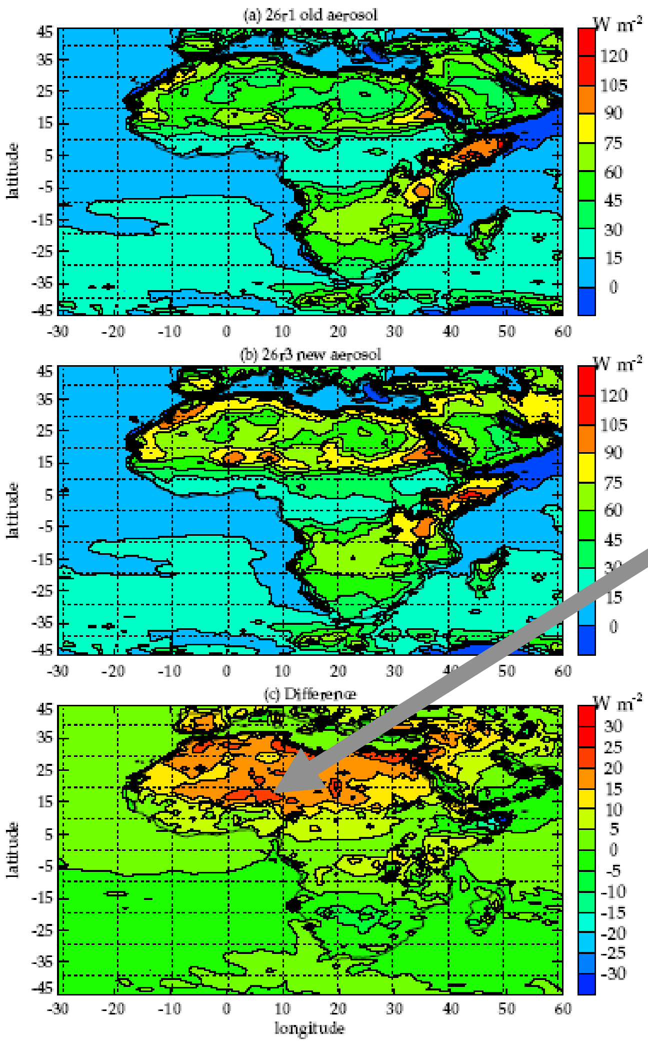
ECMWF

Impact of Aerosol Climatology on NWP

old

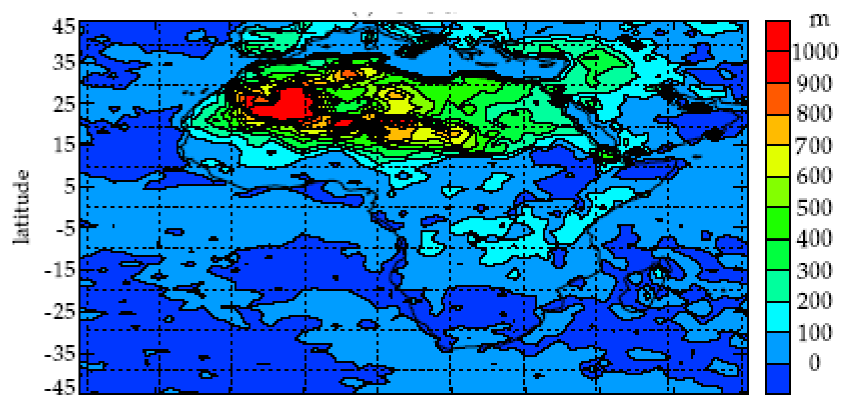
new

New-old



Surface Sensible heat flux differences

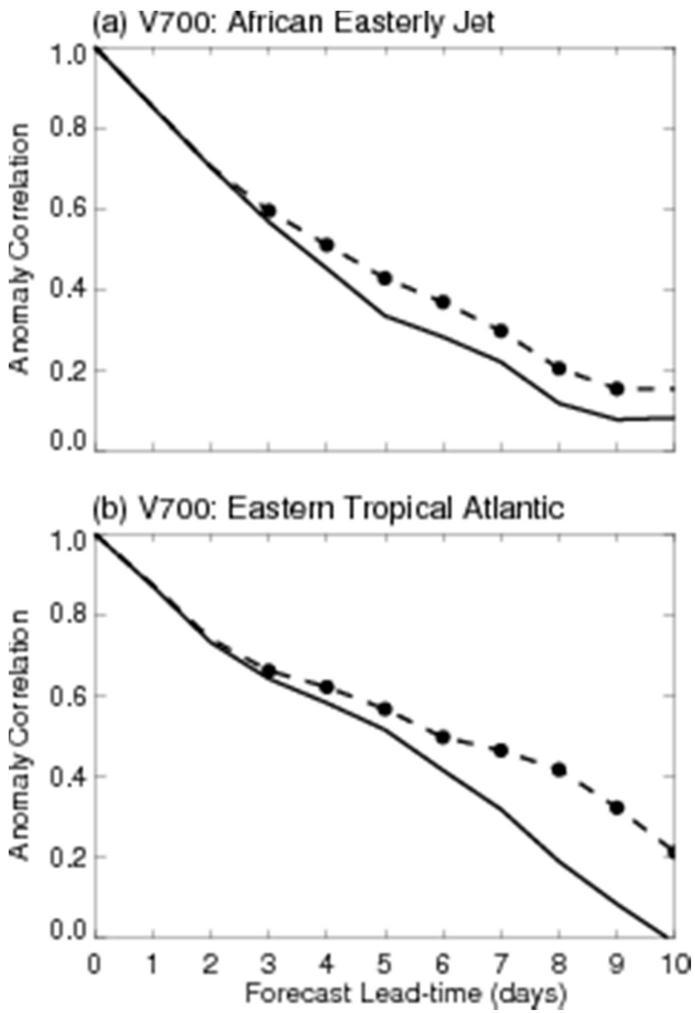
20 W m^{-2} ~ 20-30%



Boundary layer height increases >1km

Improved Predictability with improved Aerosol Climatology

New – – –
Old ——



Improved forecasts of meridional wind variations at 700 hPa for

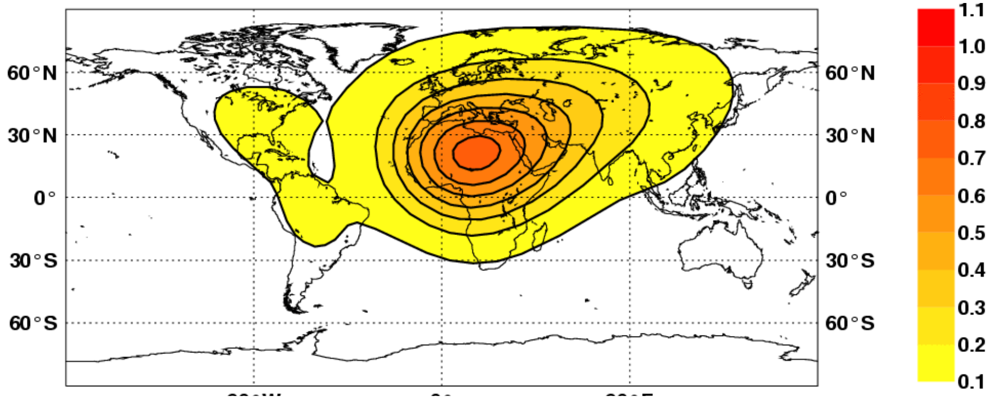
(a) the African easterly jet region and

(b) the eastern tropical Atlantic

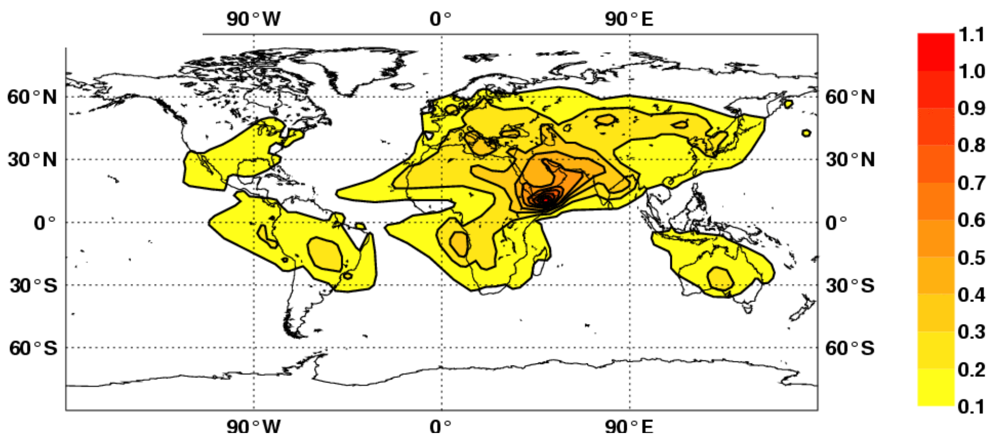
Rodwell and Jung (2008), QJRM., **134**, 1479.1497

Work in progress: Use of MACC climatology

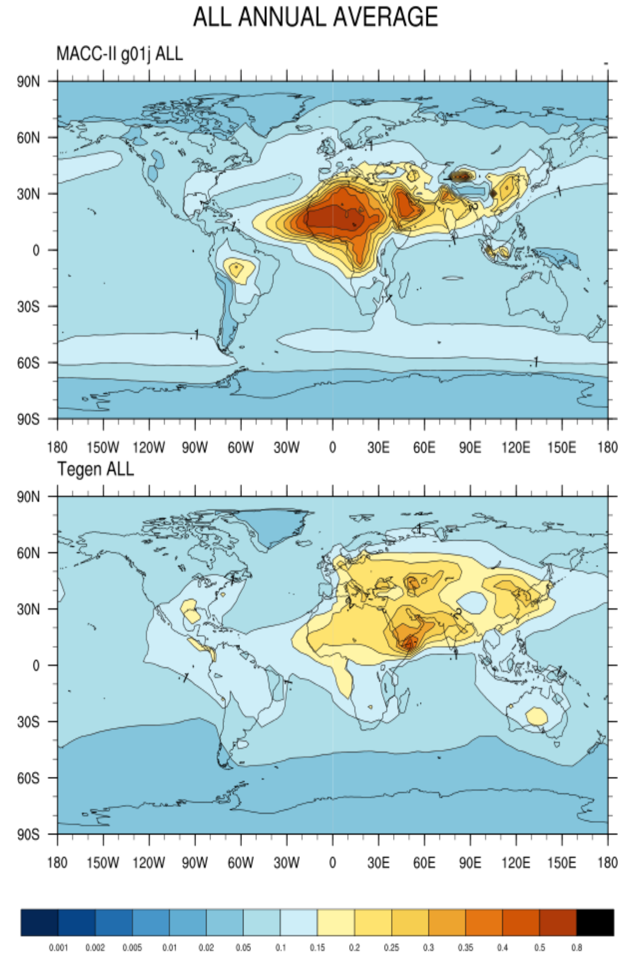
AOD 550nm



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



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



MACC

Tegen

J.-J. Morcrette
A. Tompkins

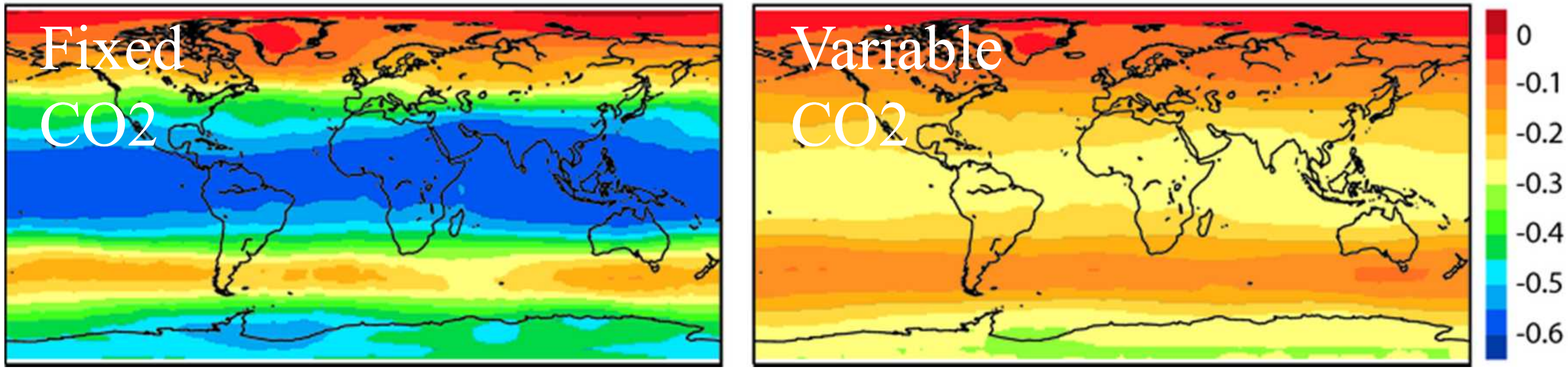
A. Bozzo

Tests are being carried out to use LW and SW aerosol prognostics in radiation code

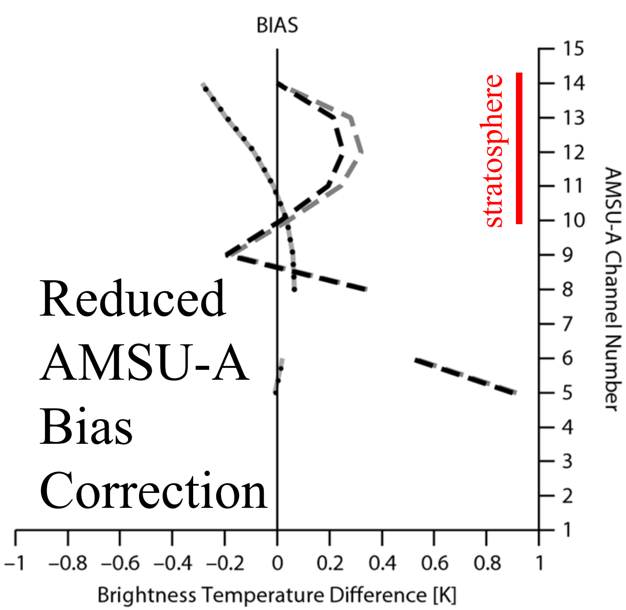
Benefit of trace gases for NWP: Variable CO_2 in radiance assimilation

Engelen and Bauer, QJRMS, 2011

Reduced AIRS and IASI Bias Correction

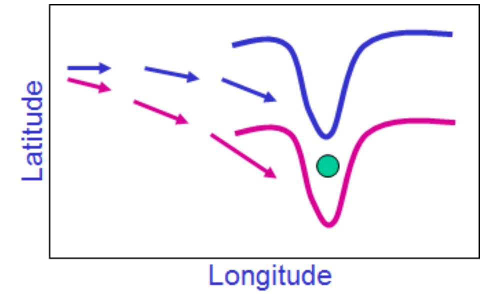


Mean bias correction (K) for August 2009 for AIRS channel 175 (699.7 cm^{-1}; maximum temperature sensitivity at ~ 200 hPa)



- 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

Wind information from tracers



- Prospect to extract wind information from long lived tracers in stratosphere and upper troposphere, e.g. O3, H2O, N2O.
- 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 H2O (Thepaut 1992) and O3 (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

Requirements to extract wind information from tracers

- Complete data coverage (3D), frequent observations
- Accurate observations
- High quality background field
- No bias between obs 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 O3 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 O3, H2O, N2O 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

Coupling between tracer and wind field in 4D-Var: illustration using 1D advection model

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:

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

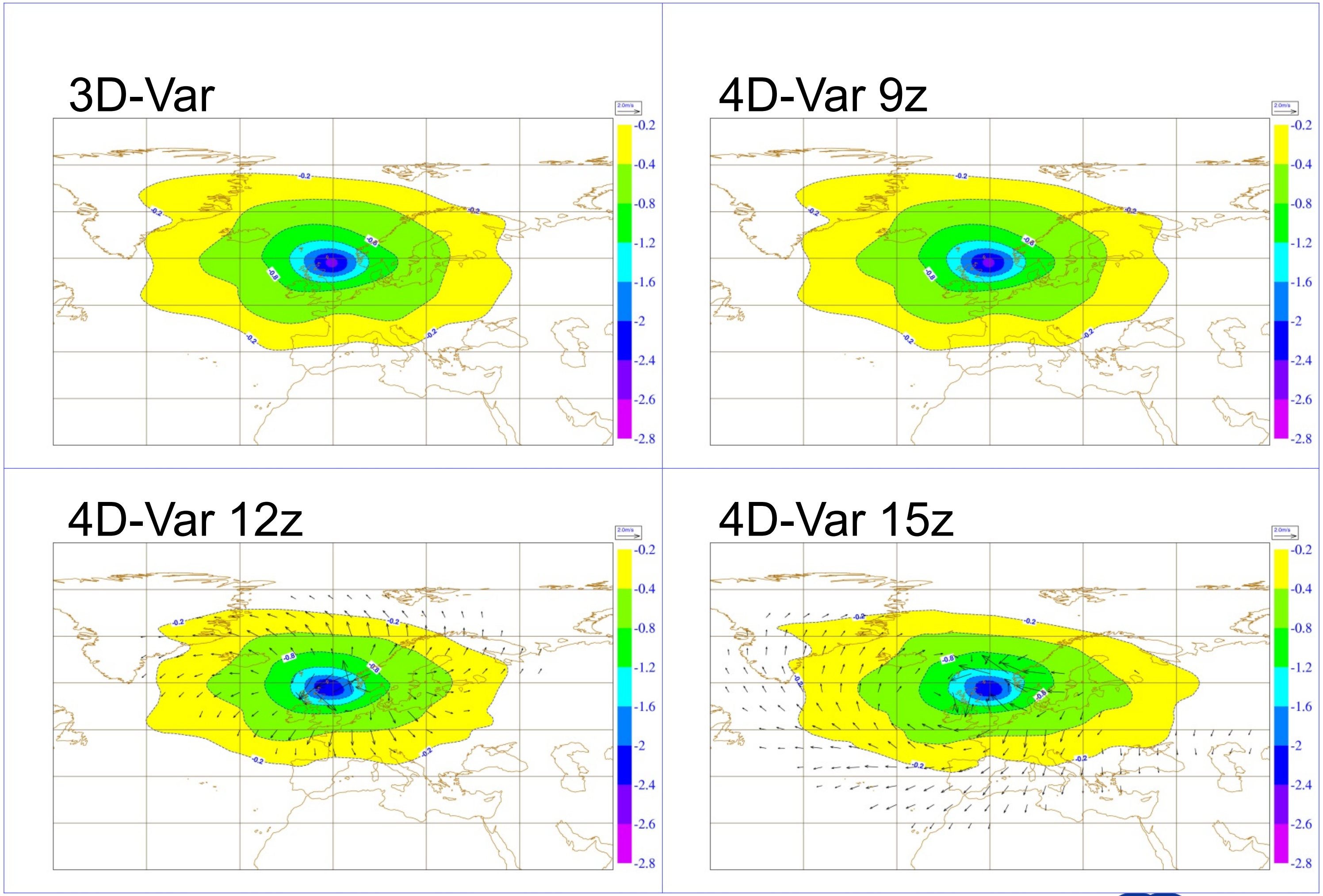
$$\frac{\partial \delta q}{\partial t} + u\frac{\partial \delta q}{\partial x} + \delta u\frac{\partial q}{\partial x} = 0$$

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

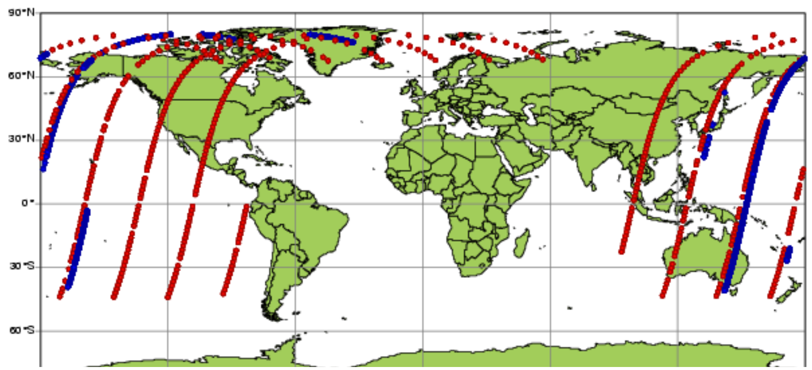


Level 20, ≈ 30 hPa

6h assimilation window

ECMWF

Impact of ozone data in 4D-Var: Example from ERA-Interim



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

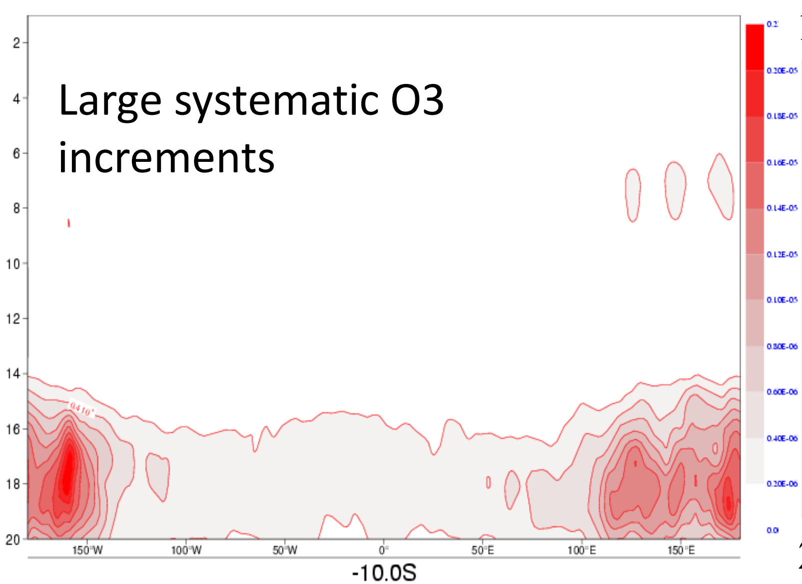
SBUV 6-layer profiles (~1,000 per day)

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

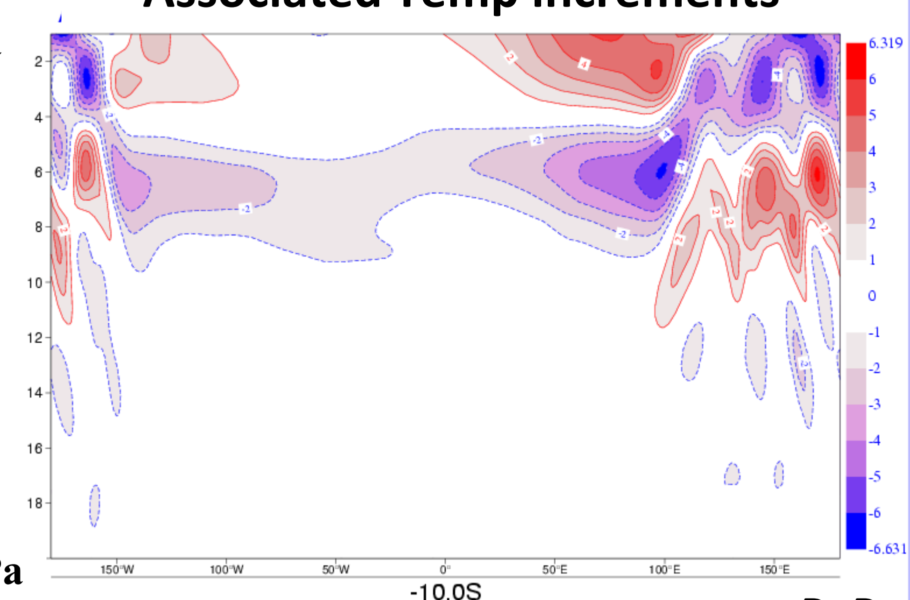
Ozone increments at 10S



1 hPa

20 hPa

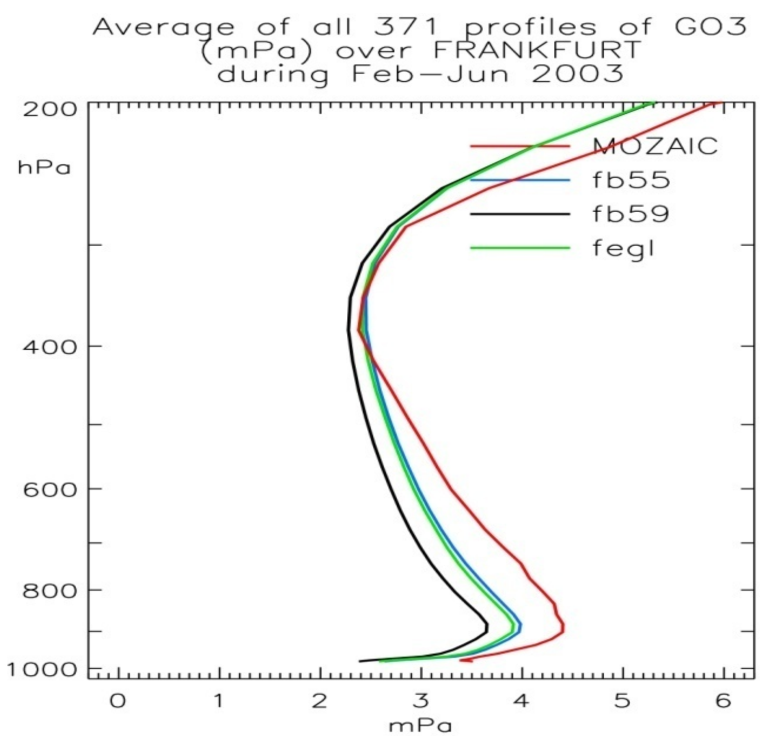
Associated Temp increments



D. Dee

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

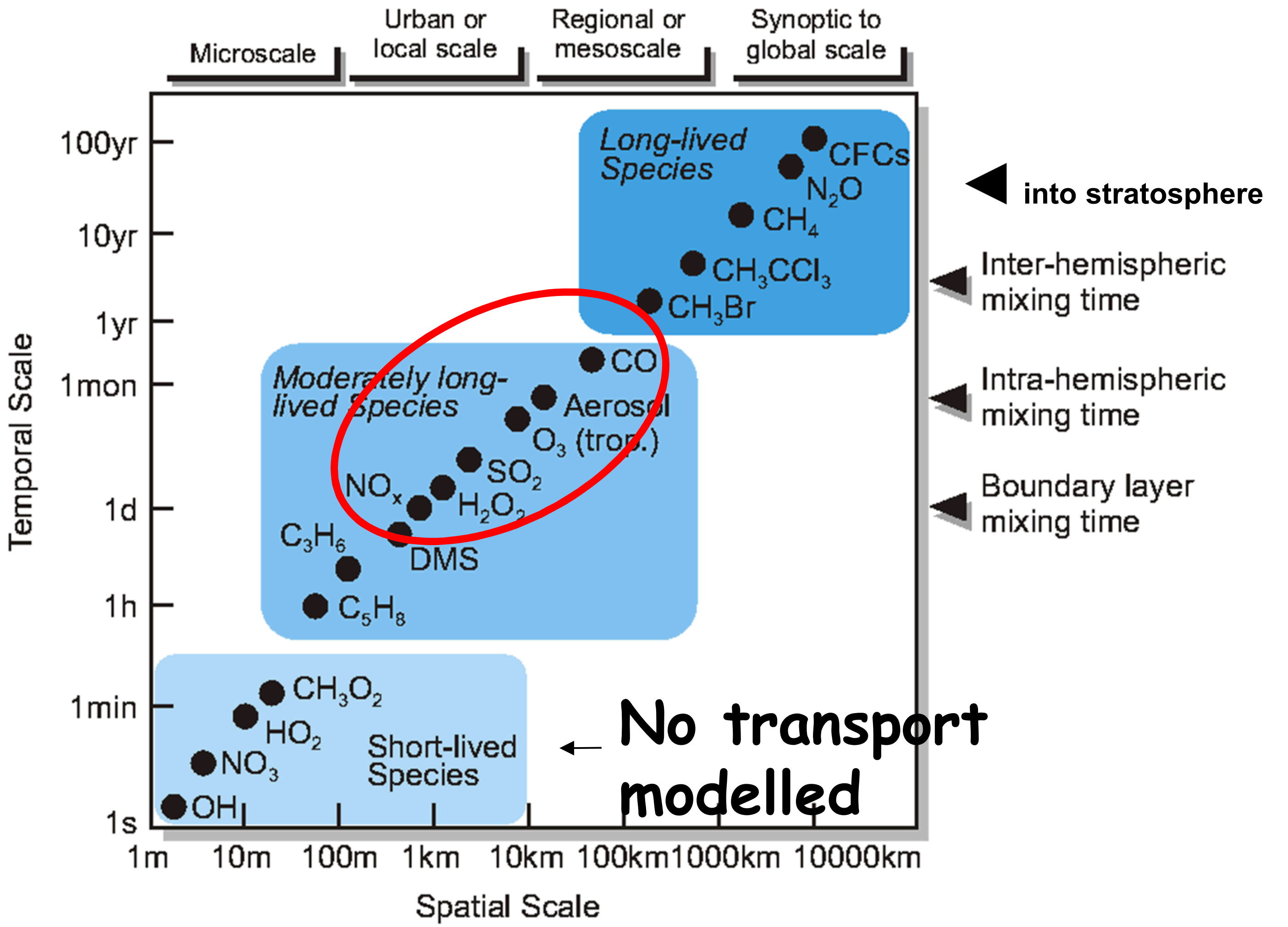
NO2 assim

3. 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
- 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,…)
- 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
- 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 (can not be measure 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)
- 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)

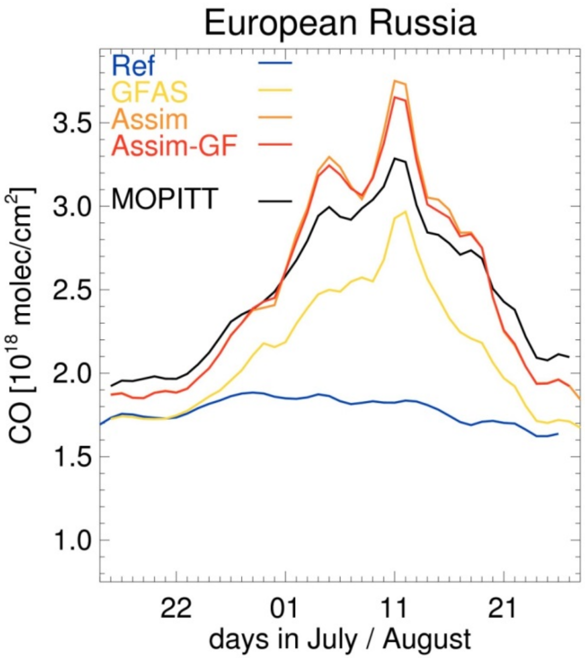
Emission Processes

- 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 (Russian fires 2010)

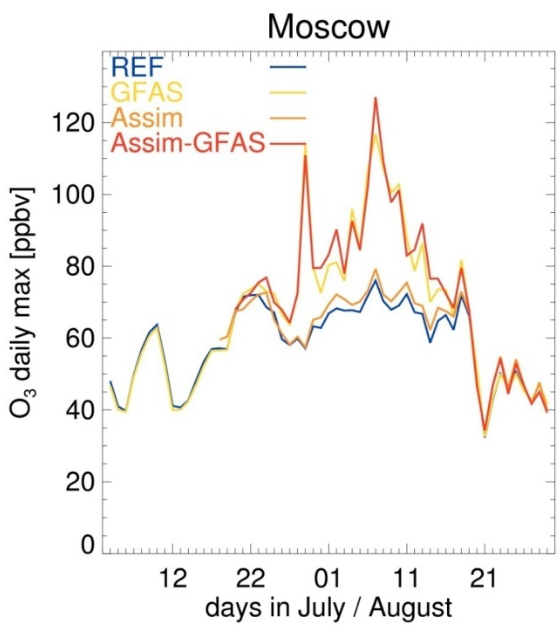
Huijnen et al. 2012 (ACP)

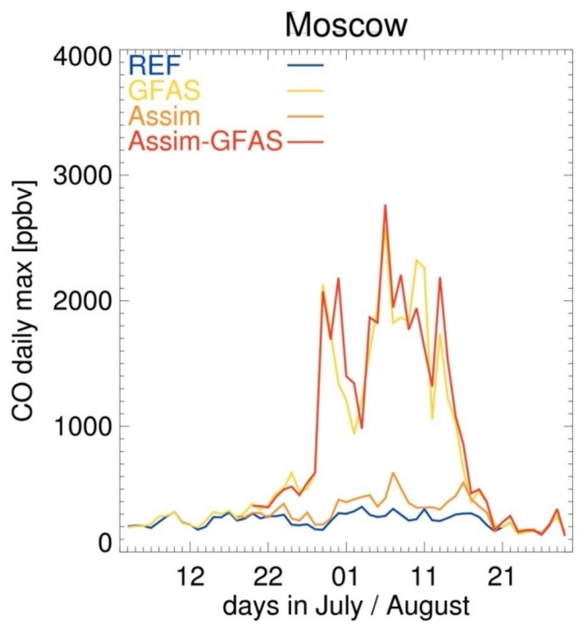
Total column CO



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

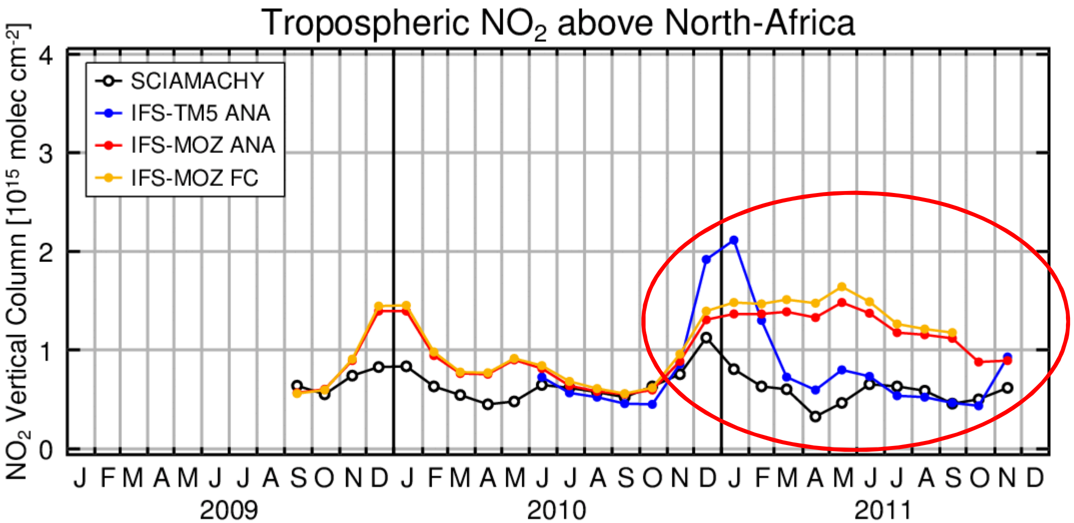
Daily maximum surface O3 and CO

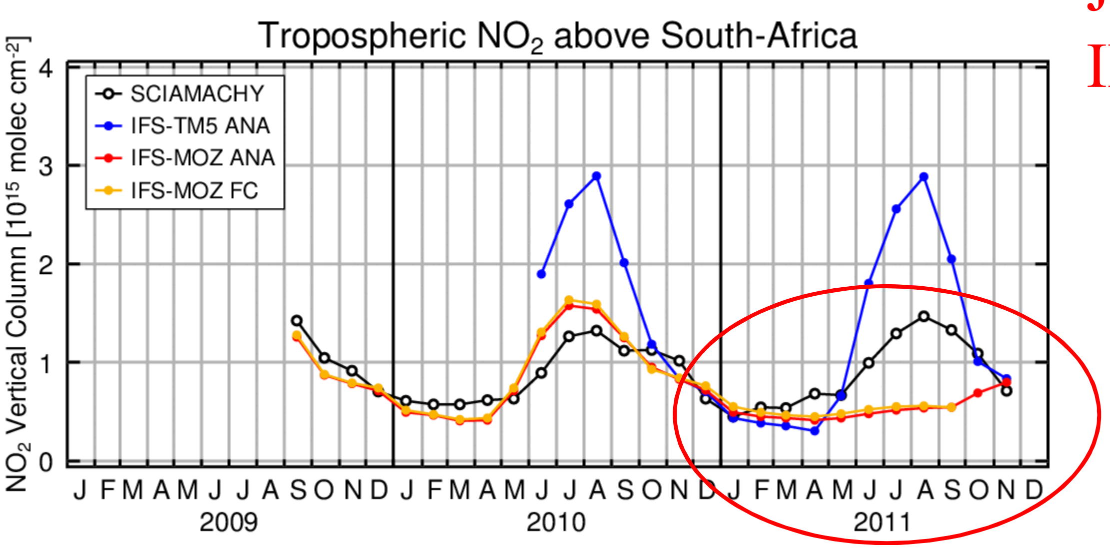




GFAS emissions are needed to get peak in surface concentrations in **GFAS** and **Assim-GFAS**

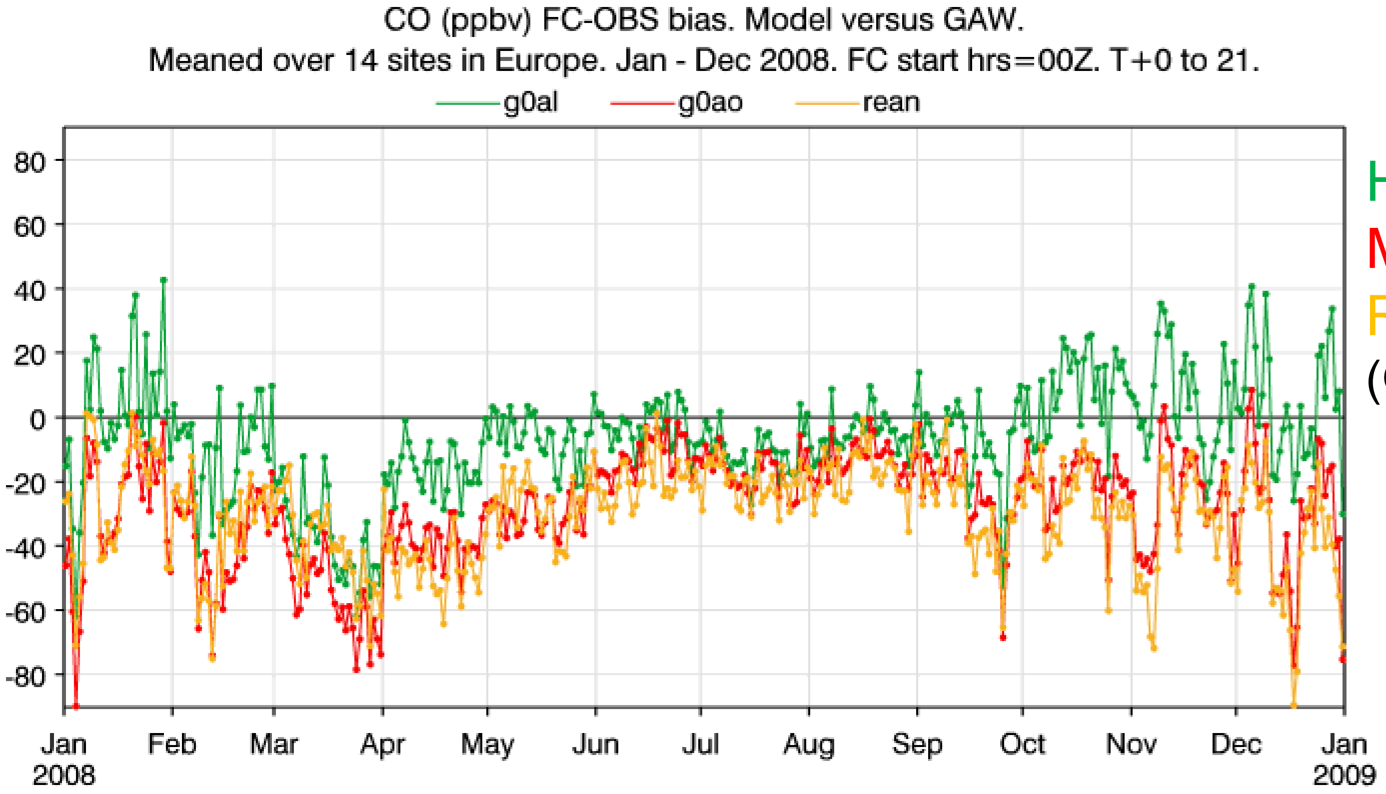
Importance of fire emissions on tropospheric NO2





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

Impact of anthropogenic emissions: CO Bias - GAW Europa timeseries



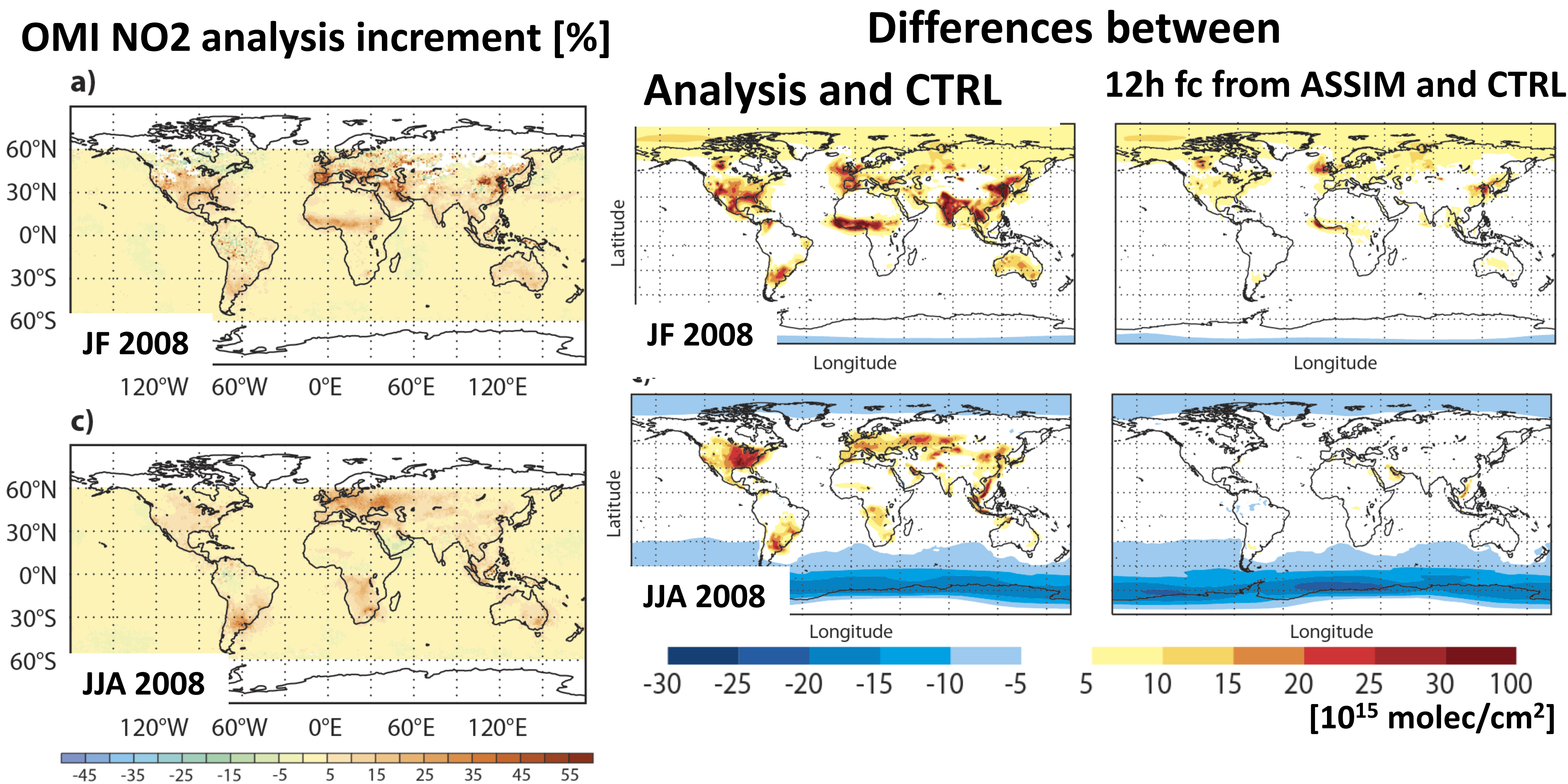
HTAP emissions
MACCity emissions
Reanalysis
(GFAS used in all runs)

Choice of emissions data set has large impact on surface concentrations

J. Flemming

ECMWF

Short lived memory of NO2 assimilation

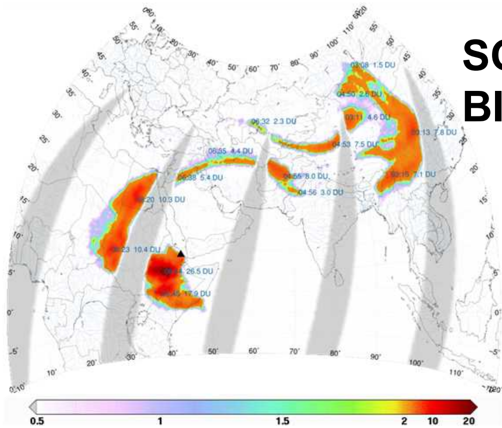


- Large positive increments from OMI NO2 assim
- Large differences between analyses of ASSIM and CTRL
- Impact is lost during subsequent 12h forecast
- It might be more beneficial to adjust emissions (instead of IC)

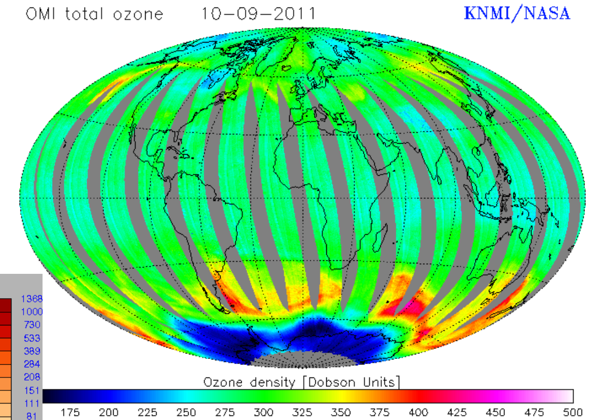
4. OBSERVATIONS OF ATMOSPHERIC COMPOSITION

Satellite observations

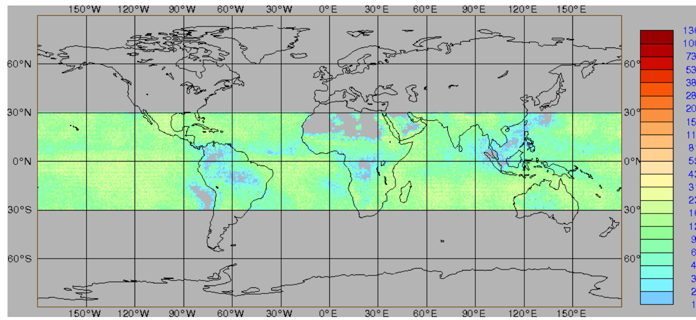
SO_2, GOME-2, SACS, BIRA/DLR/EUMETSAT



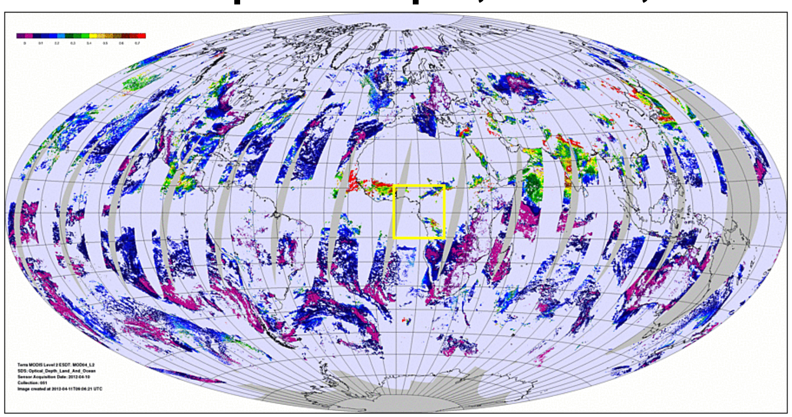
O_3, OMI, KNMI/NASA



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 …)

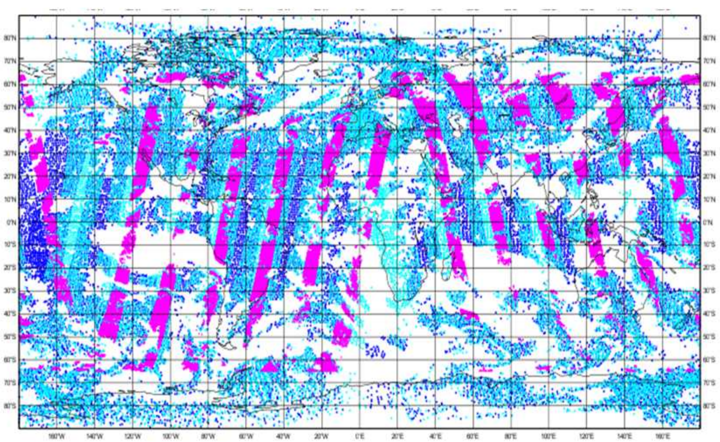
Data used in MACC NRT system (2015)

Instrument	Satellite	Satellite operator	Data provider	Species	Status
MODIS	Terra	NASA	NASA/NOAA	**Aerosol, fires**	**Active**
MODIS	Aqua	NASA	NASA/NOAA	**Aerosol, fires**	**Active**
SEVIRI	Meteosat-9	EUMETSAT	IM	**Fires**	**Active**
Imager	GOES-11, 12	NOAA	NOAA	**Fires**	**Passive**
Imager	MTSAT-2	JMA	JMA	**Fires**	Planned
MLS	Aura	NASA	NASA	**O_3**	**Active**
OMI	Aura	NASA	NASA	**O_3**	**Active**
SBUV-2	NOAA-16,19	NOAA	NOAA	**O_3**	**Active**
SCIAMACHY	Envisat	ESA	KNMI	**O_3**	**Died**
GOME-2	Metop-A	EUMETSAT	DLR	**O_3**	**Active**
GOME-2	Metop-B	EUMETSAT	DLR	**O_3**	**Active**
IASI	Metop-A	EUMETSAT	LATMOS/ULB	**CO**	**Active**
IASI	Metop-B	EUMETSAT	LATMOS/ULB	**CO**	**Active**
MOPITT	Terra	NASA	NCAR	**CO**	**Active**
GOME-2	Metop-A	EUMETSAT	DLR	**NO_2**	**Passive/Tests**
GOME-2	Metop-B	EUMETSAT	DLR	**NO_2**	**Passive/Tests**
OMI	Aura	NASA	KNMI	**NO_2**	**Active**
OMI	Aura	NASA	NASA	**SO_2**	**Active**
GOME-2	Metop-A	EUMETSAT	DLR	**SO_2**	**Active**
GOME-2	Metop-A	EUMETSAT	DLR	**SO_2**	**Active**
GOME-2	Metop-B	EUMETSAT	DLR	**HCHO**	**Passive**
TANSO-FTS	GOSAT	JAXA/NIES	UoB	**CO2**	**Active**
TANSO-FTS	GOSAT	JAXA/NIES	SRON	**CH4**	**Active**
Offline tests:					
IASI	Metop-A	EUMETSAT	LATMOS/ULB	**O3**	**Tests**

MWF

Reactive gases data availability in MACC NRT system: 20140901, 12z

CO

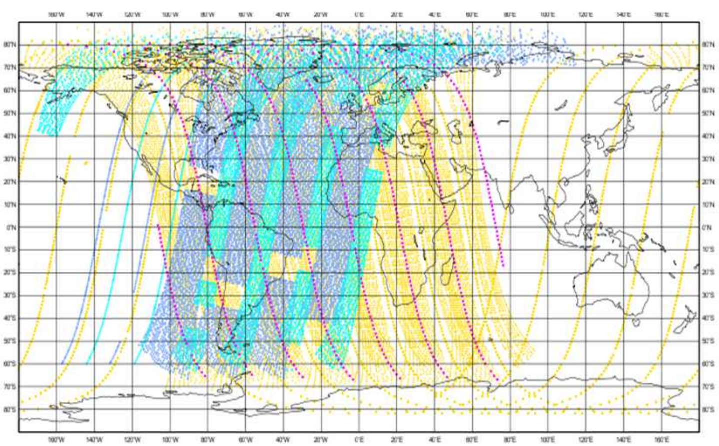


IASI Metop-A

IASI Metop-B

MOPITT TERRA

O3



GOME-2 Metop-A

GOME-2 Metop-B

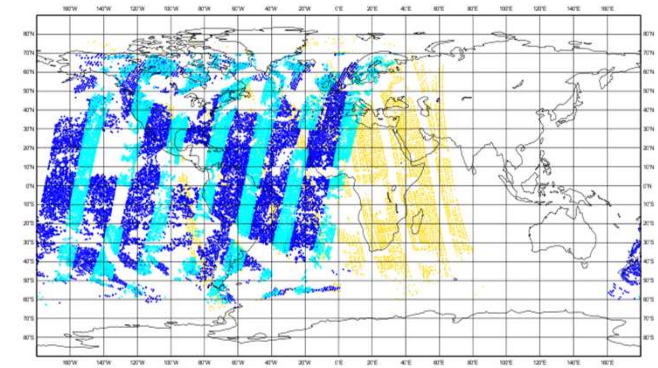
OMI, MLS AURA

SBUV/2 NOAA-19

assimilated

monitored

Tropospheric NO2

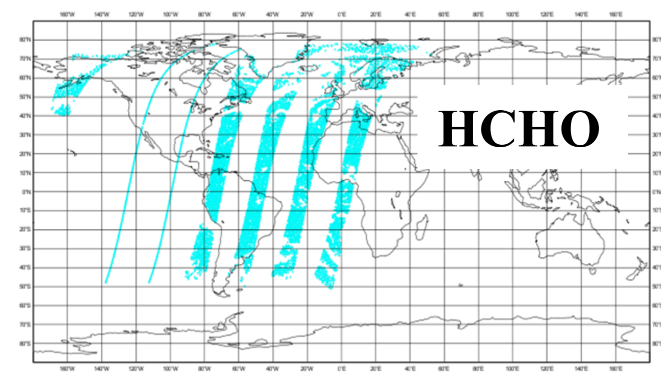


OMI AURA

GOME-2 Metop-A

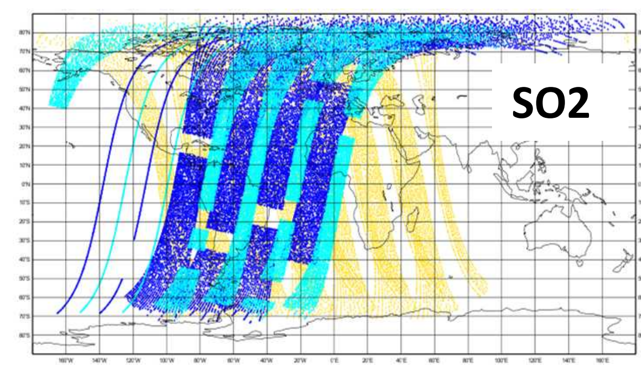
GOME-2 Metop-B

HCHO



GOME-2 Metop-A

SO2



OMI AURA

GOME-2 Metop-A

GOME-2 Metop-B

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)

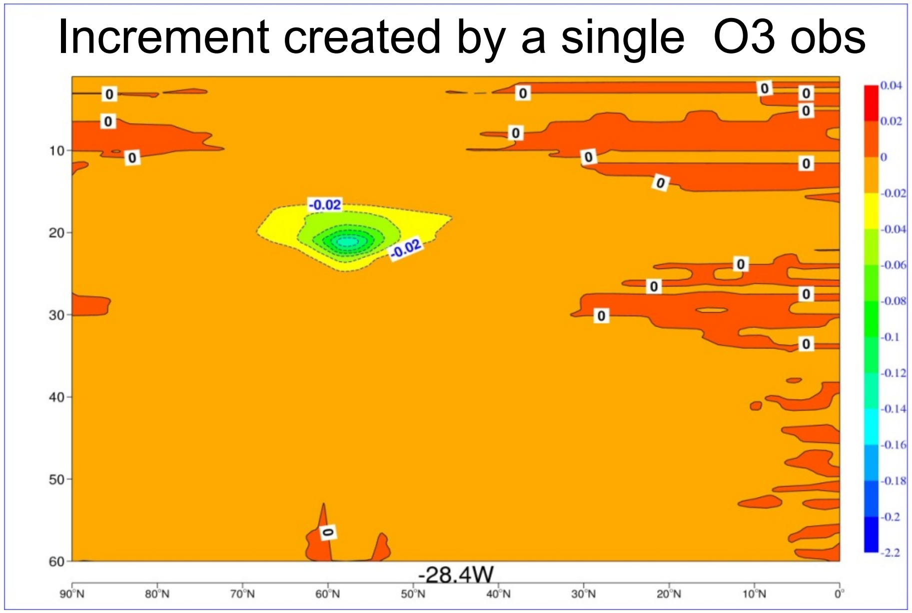
$$x_a - x_b = \frac{y - x_b}{\sigma_o^2 + \sigma_b^2} B$$

- 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

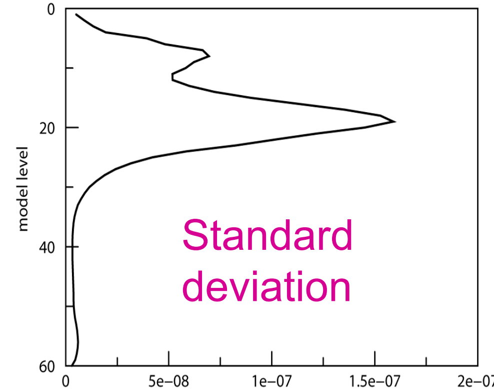
- Analysis increment is proportional to a column of B-matrix
- B-matrix determines how increment is spread out from a single observation to neighbouring gridpoints/ levels

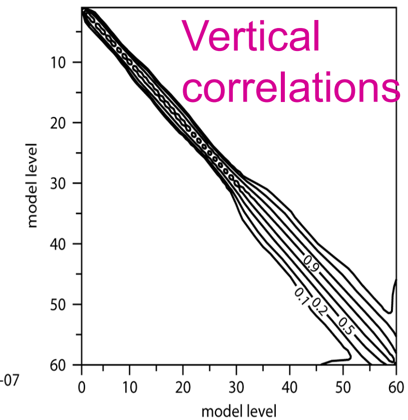
Increment from a single TCO3 observation

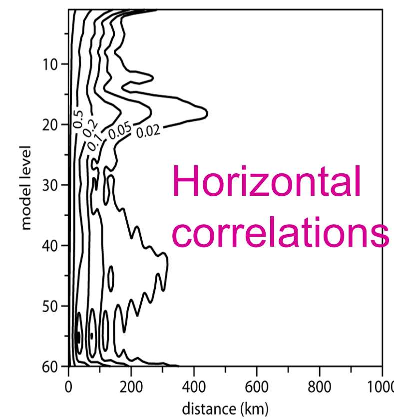
Ozone background errors



Ozone observation of 247 DU, 66 DU lower than background

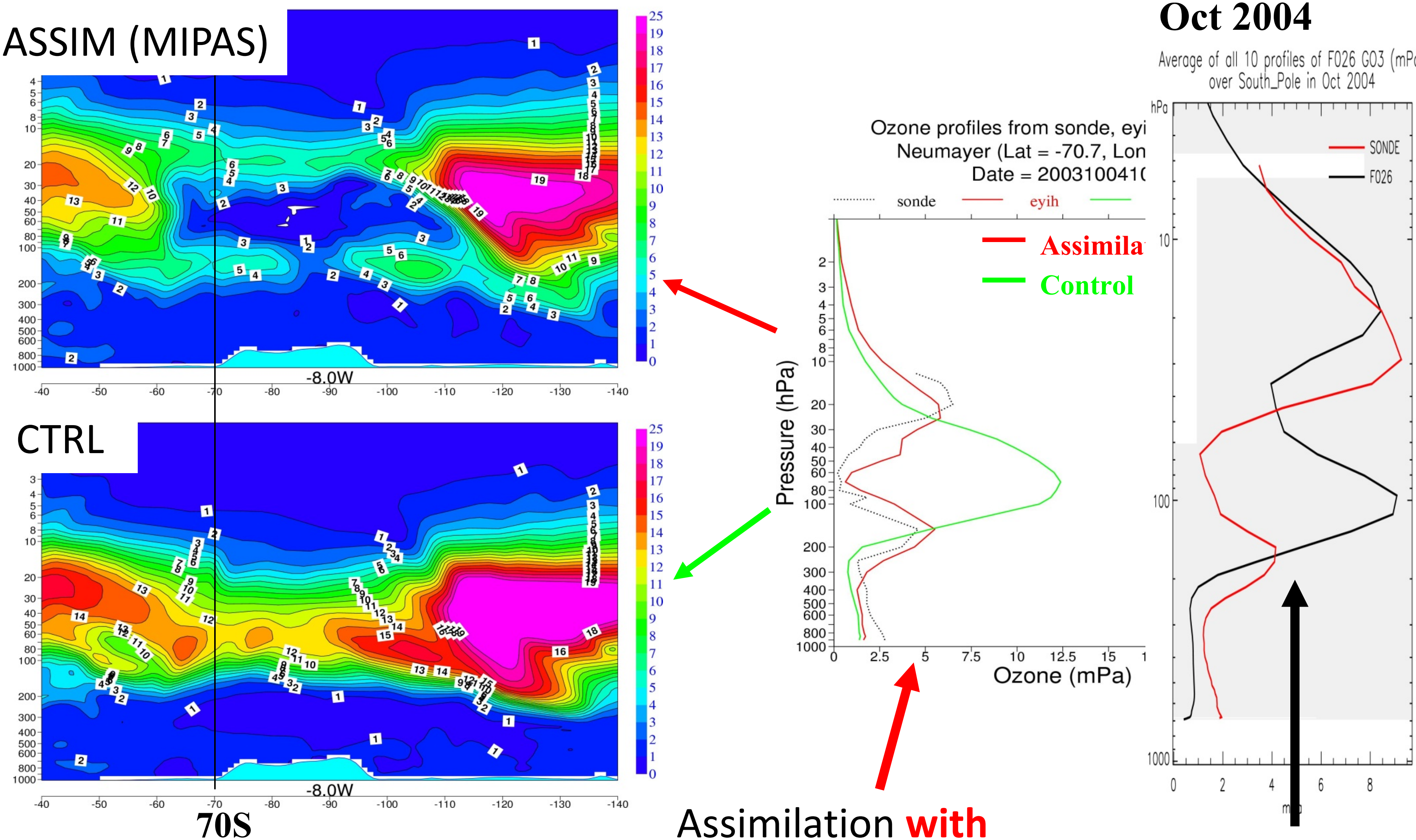






- Maximum impact around L20 (~35 hPa)
- Profile data are important to obtain a good vertical analysis profiles

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



Assimilation **with profile data**

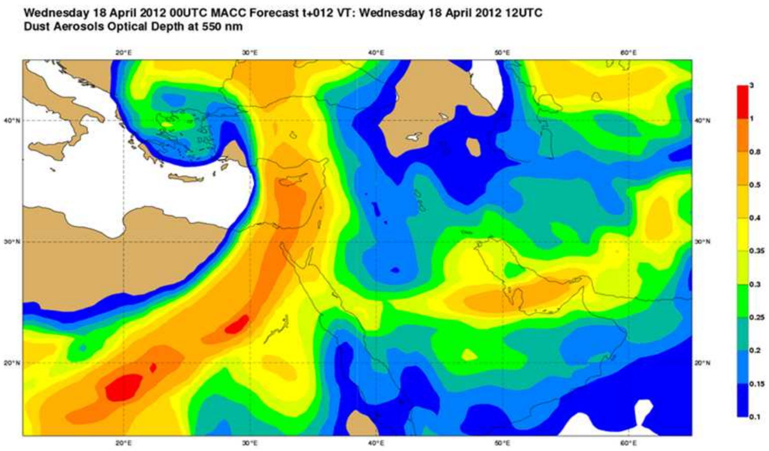
Assimilation **with total column data**

5. 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:

fine mode
coarse mode

* 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 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.
- Improvements of dual mode control variable are especially seen in fine mode AOD
- Analysis increments are repartitioned into the species according to their fractional contribution to the total or fine/coarse mode aerosol 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.

Angela Benedetti

How does it work?

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.

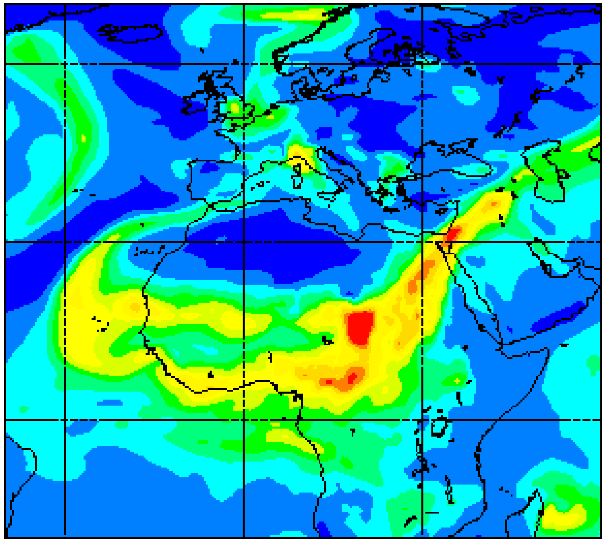
3. The gradient wrt total aerosol mixing ratio is then used in the minimization and the resulting increment in r_t is used in the tangent linear run to compute updated perturbations on the individual bin/species mixing ratios as follows:

$$r_i' = f_i r_t'$$

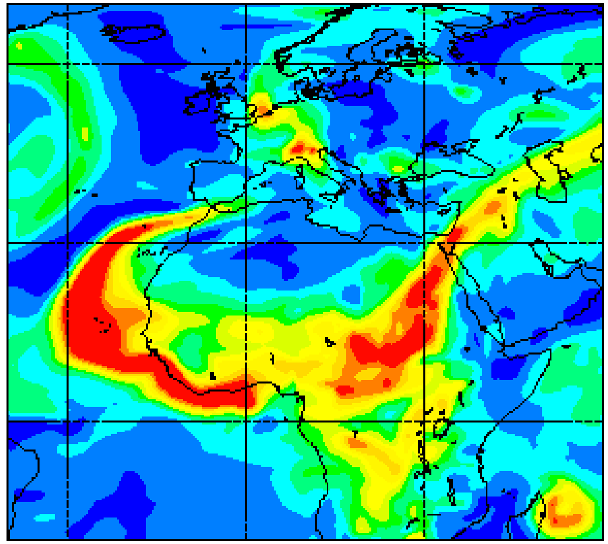
This last step is not fully justifiable unless $r_t = \sum_i r_i$ at all times and at all locations.

Saharan dust outbreak: 6 March 2004

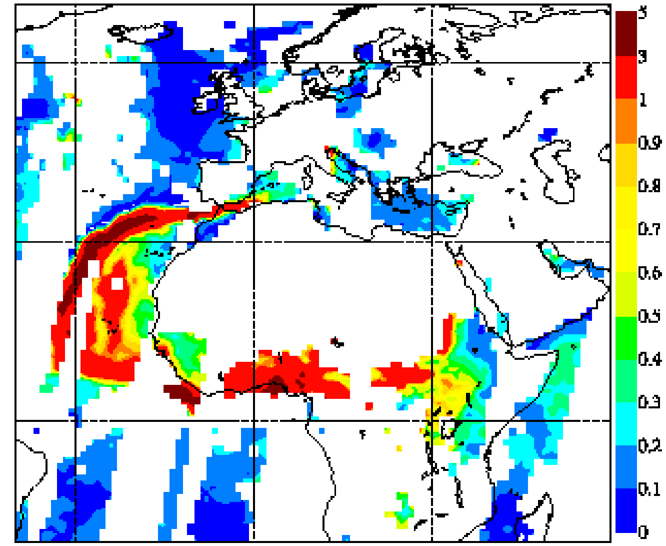
Model simulation



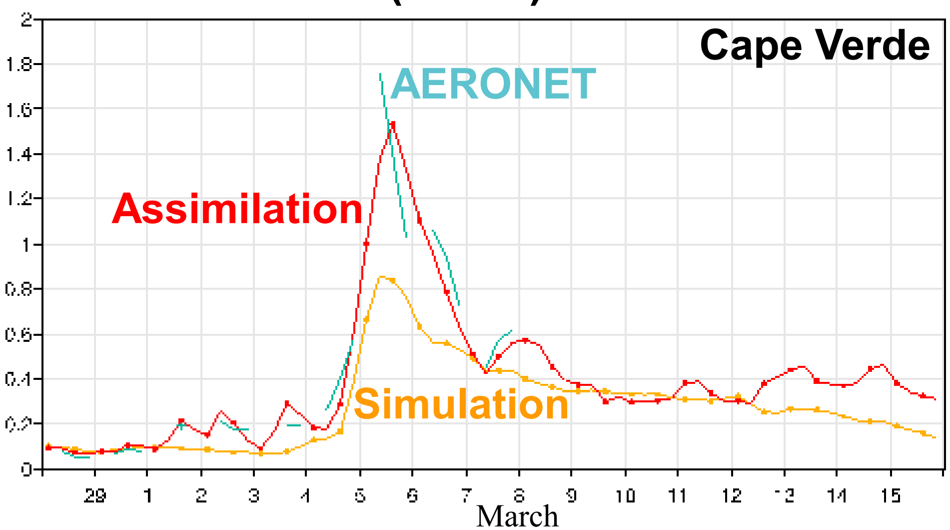
Assimilation

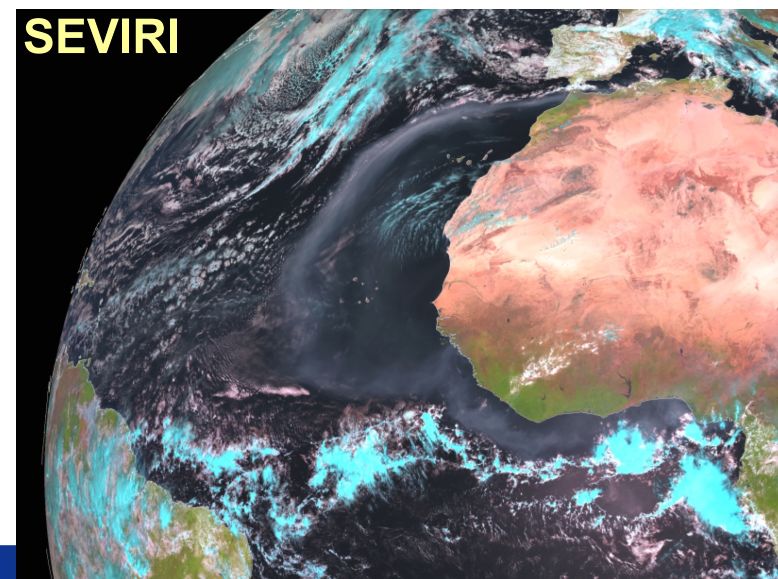


MODIS



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

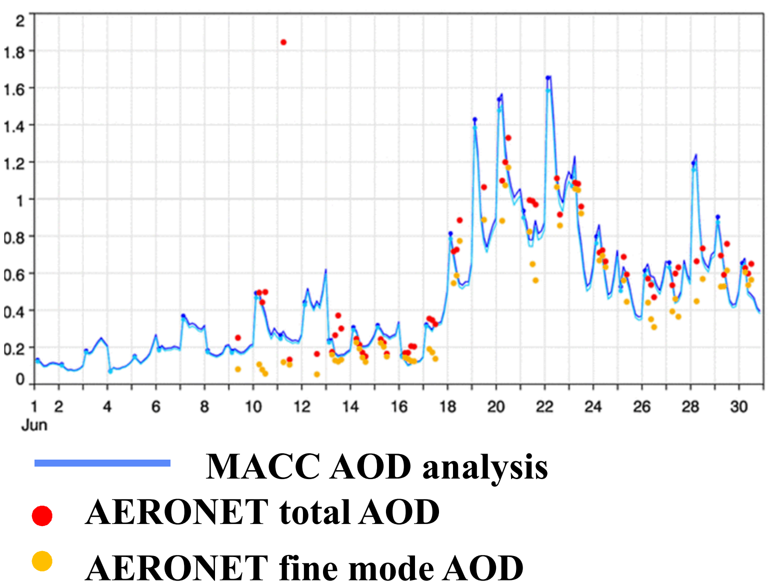


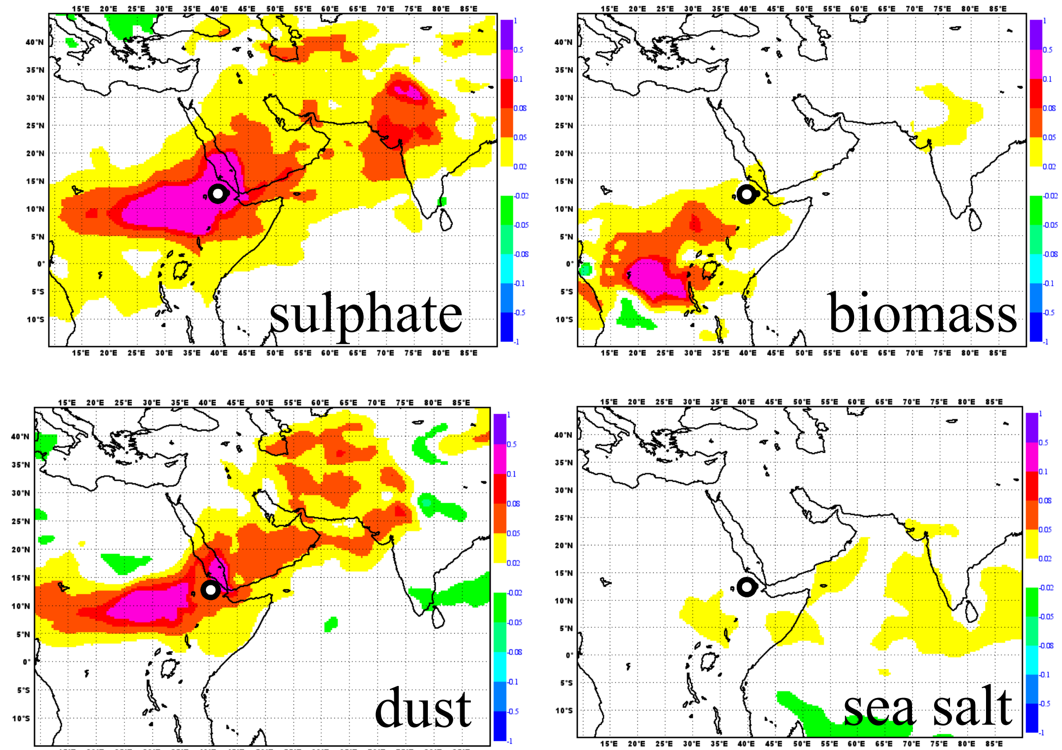


Example for wrong aerosol attribution

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

ICIPE-Mbita - AERONET

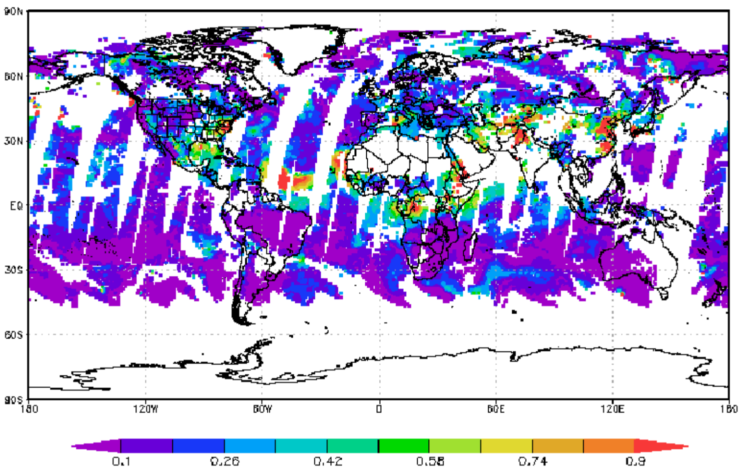


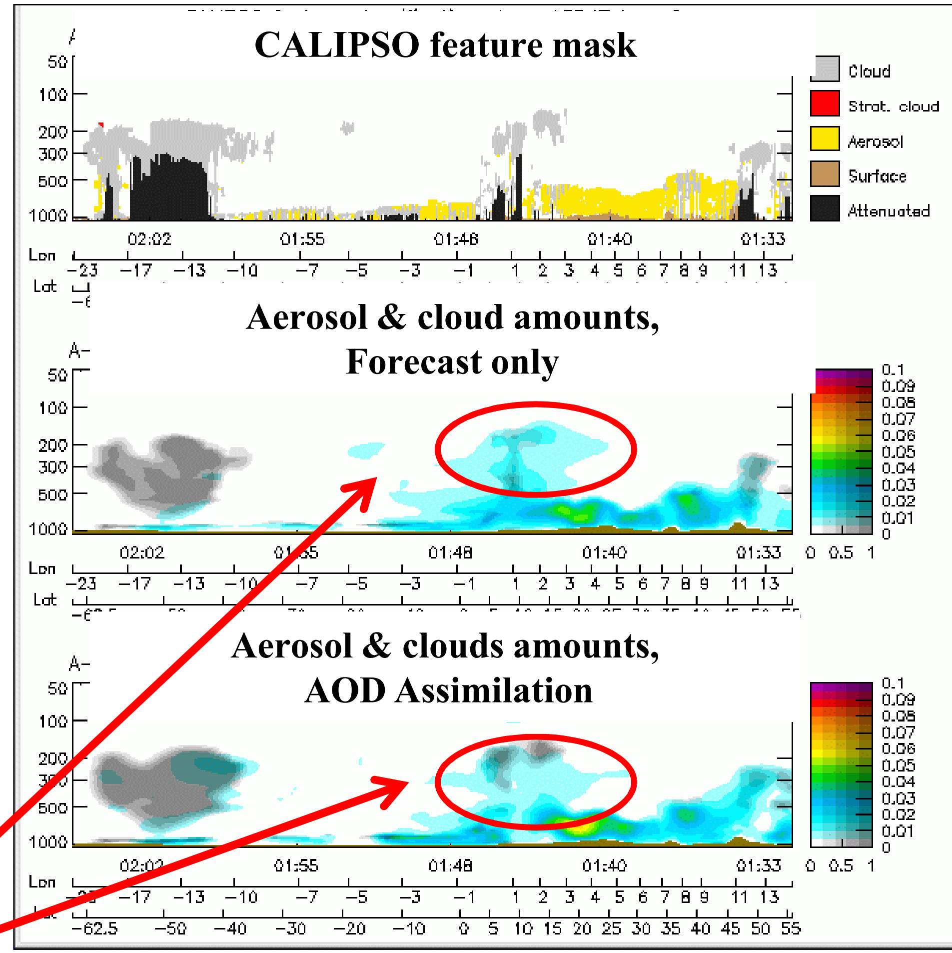


The MACC aerosol model did not contain stratospheric aerosol at this time, so the observed AOD was wrongly attributed to the available aerosol types.

Why we need profiling data for aerosol assimilation

MODIS Aerosol Optical Depth





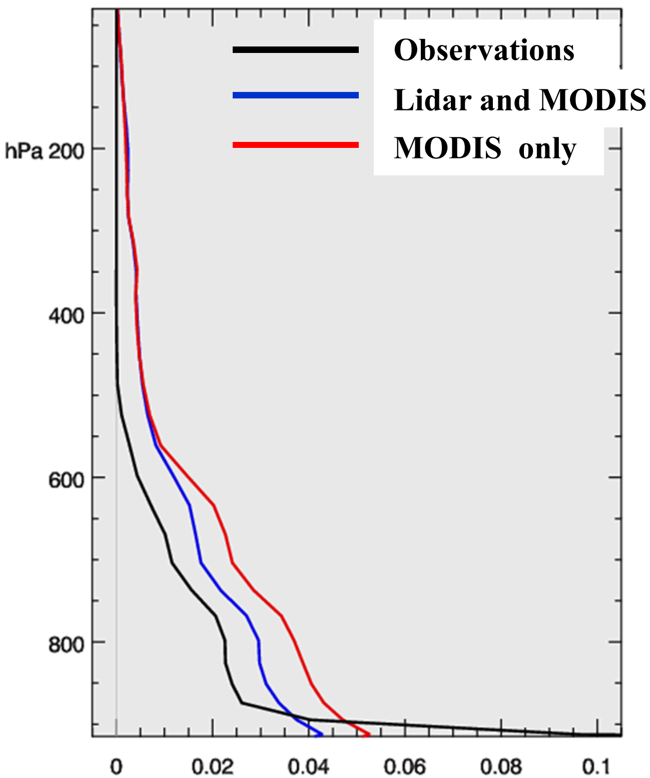
- AOD is a column-integrated quantity
- Assimilation of AOD does not modify the vertical profile
- Profile data are needed (lidar)

Graphics by Luke Jones

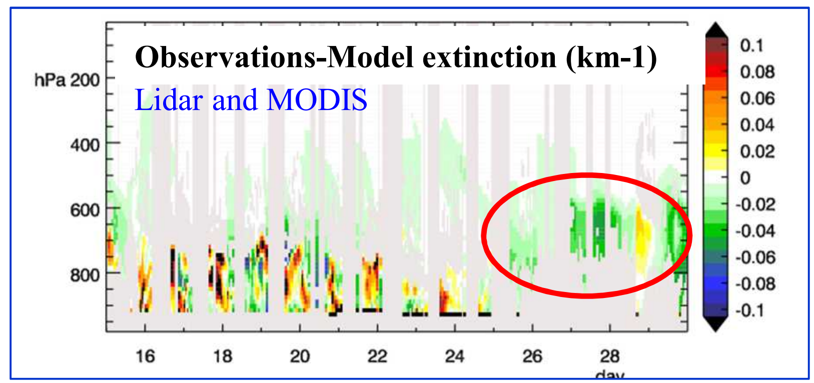
ECMWF

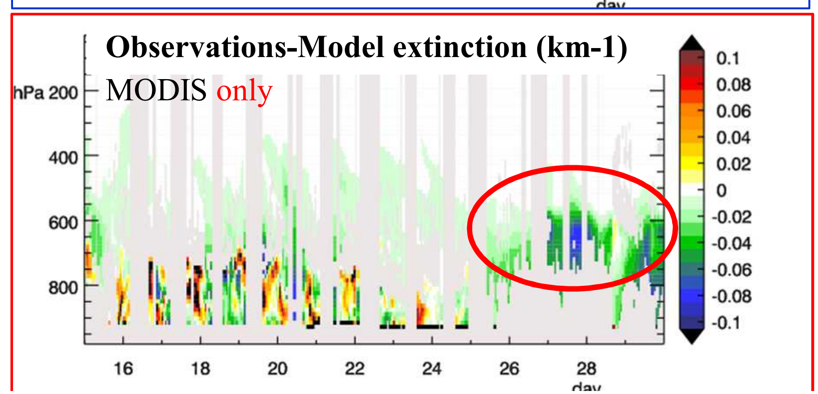
Towards lidar assimilation: Impact of Calipso on vertical profiles

- 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.

6. Concluding remarks

- Atmospheric composition (AC) and weather interact
- IFS has been extended to include fields of atmospheric composition: Reactive gases, greenhouse gases, aerosols => **Composition-IFS (C-IFS)**
- Modelling of AC needs to include many species with concentrations varying over several orders of magnitude
- AC forecasts benefit from realistic initial conditions (**data assimilation**) but likewise from improved emissions
- Extra challenges for DA of atmospheric composition compared to NWP - but also potential benefits through chemical coupling and impact on NWP
- MACC/ CAMS system produces useful AC forecast and analyses, freely available from www.copernicus-atmosphere.eu

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

http://www.copernicus-atmosphere.eu

For questions contact:

info@copernicus-atmosphere.eu

References: Reactive Gases

N. Elguindi, H. Clark, C. Ordóñez, V. Thouret, J. Flemming, O. Stein, V. Huijnen, P. Moinat, A. Inness, V.-H. Peuch, A. Stohl, S. Turquety, G. Athier, J.-P. Cammas, and M. Schultz (2010): Current status of the ability of the GEMS/MACC models to reproduce the tropospheric CO vertical distribution as measured by MOZAIC. Geosci. Model Dev., 3, 501-518, 2010

Flemming, J., Huijnen, V., Arteta, J., Bechtold, P., Beljaars, A., Blechschmidt, A.-M., Josse, B., Diamantakis, M., Engelen, R. J., Gaudel, A., Inness, A., Jones, L., Katragkou, E., Marecal, V., Peuch, V.-H., Richter, A., Schultz, M. G., Stein, O., and Tsikerdekis, A.: Tropospheric chemistry in the integrated forecasting system of ECMWF, Geosci. Model Dev. Discuss., 7, 7733-7803, doi:10.5194/gmdd-7-7733-2014, 2014.

Flemming, J., and A. Inness (2013), Volcanic sulfur dioxide plume forecasts based on UV satellite retrievals for the 2011 Grímsvötn and the 2010 Eyjafjallajökull eruption, J. Geophys. Res. Atmos., 118, doi:10.1002/jgrd.50753.

Flemming, J., Inness, A., Jones, L., Eskes, H. J., Huijnen, V., Schultz, M. G., Stein, O., Cariolle, D., Kinnison, D., and Brasseur, G. (2011): Forecasts and assimilation experiments of the Antarctic ozone hole 2008, Atmos. Chem. Phys., 11, 1961-1977, doi:10.5194/acp-11-1961-2011

J. Flemming, Inness, A., Flentje, H., Huijen, V., Moinat, P., Schultz, M.G. and Stein O. (2009): Coupling global chemistry transport models to ECMWF's integrated forecast system. Geosci. Model Dev., 2, 253-265, 2009. www.geosci-model-dev.net/2/253/2009/

Huijnen, V., Flemming, J., Kaiser, J. W., Inness, A., Leitao, J., Heil, A., Eskes, H. J., Schultz, M. G., Benedetti, A., Hadji-Lazaro, J., Dufour, G., and Eremenko, M. (2012). Hindcast experiments of tropospheric composition during the summer 2010 fires over western Russia. Atmos. Chem. Phys., 12:4341–4364.

References: Reactive Gases

Inness, A., Blechschmidt, A.-M., Bouarar, I., Chabrillat, S., Crepulja, M., Engelen, R. J., Eskes, H., Flemming, J., Gaudel, A., Hendrick, F., Huijnen, V., Jones, L., Kapsomenakis, J., Katragkou, E., Keppens, A., Langerock, B., de Mazière, M., Melas, D., Parrington, M., Peuch, V. H., Razinger, M., Richter, A., Schultz, M. G., Suttie, M., Thouret, V., Vrekoussis, M., Wagner, A., and Zerefos, C.: Data assimilation of satellite retrieved ozone, carbon monoxide and nitrogen dioxide with ECMWF's Composition-IFS, Atmos. Chem. Phys. Discuss., 15, 4265-4331, doi:10.5194/acpd-15-4265-2015, 2015.

Inness, A., Baier, F., Benedetti, A., Bouarar, I., Chabrillat, S., Clark, H., Clerbaux, C., Coheur, P., Engelen, R. J., Errera, Q., Flemming, J., George, M., Granier, C., Hadji-Lazaro, J., Huijnen, V., Hurtmans, D., Jones, L., Kaiser, J. W., Kapsomenakis, J., Lefever, K., Leita˜o, J., Razinger,M., Richter, A., Schultz, M. G., Simmons, A. J., Suttie, M., Stein, O., Th´epaut, J.-N., Thouret, V., Vrekoussis, M., Zerefos, C., and the MACC team (2013). The MACC reanalysis: an 8 yr data set of atmospheric composition. Atmos. Chem. Phys., 13(8):4073–4109.

Inness, A., Flemming, J., Suttie, M. and Jones, L., 2009: GEMS data assimilation system for chemically reactive gases. ECMWF RD Tech Memo 587. Available from http://www.ecmwf.int.

C. Ordonez, N. Elguindi, O. Stein, V. Huijnen, J. Flemming, A. Inness, H. Flentje, E. Katragkou, P. Moinat, V-H. Peuch, A. Segers, V. Thouret, G. Athier, M. van Weele, C. S. Zerefos, J-P. Cammas, and M. G. Schultz (2009): Global model simulations of air pollution during the 2003 European heat wave. Atmos. Chem. Phys., 10, 789-815, 2010. www.atmos-chem-phys.net/10/789/2010/

Stein, O., Flemming, J., Inness, A., Kaiser, J. W., and Schultz, M. G. (2012). Global re- active gases forecasts and reanalysis in the MACC project. Journal of Integrative Environmental Sciences, 1:1–14

References: Areosols

Bellouin, N., J. Quaas, J.-J. Morcrette, and O. Boucher, 2013: Estimates of radiative forcing from the MACC re-analysis. Atmos. Chem. Phys., 13, 2045-2062.

Benedetti, A. et al, 2014: Operational dust prediction. Chapter 10 in: Knippertz, P.; Stuut, J.-B. (eds.), Mineral Dust – A Key Player in the Earth System, Springer Netherlands, 223–265, ISBN 978-94-017-8977-6. doi:10.1007/978-94-017-8978-3_10

Benedetti, A., Morcrette, J.-J., Boucher, O., Dethof, A., Engelen, R. J., Fisher, M., Flentje, H., Huneeus, N., Jones, L., Kaiser, J. W., Kinne, S., Manglold, A., Razinger, M., Simmons, A. J., and Suttie, M. (2009). Aerosol analysis and forecast in the European Centre for Medium-Range Weather Forecasts Integrated Forecast System: 2. Data assimilation. J. Geophys. Res., 114(D13):D13205

Benedetti, A., Kaiser, J. W., and Morcrette, J.-J. (2012). Global aerosols [in “State of the climate in 2011”]. Bull. Amer. Meteor. Soc., 93(7):S44–S46. (Also for other years)

Huneeus, N., M. Schulz, Y. Balkanski, J. Griesfeller, S. Kinne, J. Prospero, S. Bauer, O. Boucher, M. Chin, F. Dentener, T. Diehl, R. Easter, D. Fillmore, S. Ghan, P. Ginoux, A. Grini, L. Horowitz, D. Koch, M.C. Krol, W. Landing, X. Liu, N. Mahowald, R. Miller, J.-J. Morcrette, G. Myhre, J. Penner, J. Perlwitz, P. Stier, T. Takemura, and C. Zender, 2011: Global dust model intercomparison in AEROCOM phase I. Atmos. Chem. Phys., 11, 7781-7816, doi:10.5194/acp-11-7781-2011.

Mangold, A., H. De Backer, B. De Paepe, S. Dewitte, I. Chiapello, Y. Derimian, M. Kacenelenbogen, J.-F. Léon, N. Huneeus, M. Schulz, D. Ceburnis, C. O'Dowd, H. Flentje, S. Kinne, A. Benedetti, J.-J. Morcrette, and O. Boucher, 2011: Aerosol analysis and forecast in the European Centre for Medium-Range Weather Forecasts Integrated Forecast System: 3. Evaluation by means of case studies, J. Geophys. Res.,116, D03302, doi: 10.1029 /2010JD014864.

References: Areosols

Morcrette, J.-J., Boucher, O., Jones, L., Salmond, D., Bechtold, P., Beljaars, A., Benedetti, A., Bonet, A., Kaiser, J. W., Razinger, M., Schulz, M., Serrar, S., Simmons, A. J., Sofiev, M., Suttie, M., Tompkins, A. M., and Untch, A. (2009). Aerosol analysis and forecast in the European Centre for Medium-Range Weather Forecasts Integrated Forecast System: Forward modeling. J. Geophys. Res., 114(D6):D06206.

Morcrette, J.-J., O. Boucher, L. Jones, D. Salmond, P. Bechtold, A. Beljaars, A. Benedetti, A. Bonet, J.W. Kaiser, M. Razinger, M. Schulz, S. Serrar, A.J. Simmons, M. Sofiev, M. Suttie, A.M. Tompkins, A. Untch, and the GEMS-AER team, 2009: Aerosol analysis and forecast in the ECMWF Integrated Forecast System: Forward modelling. J. Geophys. Res., 114, D06206, doi: 10.1029 /2008JD011235.

Morcrette, J.-J., A. Beljaars, A. Benedetti, L. Jones, and O. Boucher, 2008: Sea-salt and dust aerosols in the ECMWF IFS. Geophys. Res. Lett., 35, L24813, doi:10.1029/2008GL036041.

Morcrette, J.-J., A. Benedetti, L. Jones, J.W. Kaiser, M. Razinger, and M. Suttie, 2011: Prognostic aerosols in the ECMWF IFS: MACC vs. GEMS aerosols. ECMWF Technical Memorandum, 659, 32 pp.

Morcrette, J.-J., A. Benedetti, A. Ghelli, J.W. Kaiser, and A.P. Tompkins, 2011: Aerosol-cloud-radiation interactions and their impact on ECMWF/MACC forecasts. ECMWF Technical Memorandum, 660, 35 pp.

Nabat, P., S. Somot, M. Mallet, I. Chiapello, J.-J. Morcrette, F. Solmon, S. Szopa, and F. Dulac, 2013: A 4-D climatology (1979-2009) of the monthly aerosol optical depth distribution over the Mediterranean and surrounding regions from a comparative evaluation and blending of remote sensing and model products. Atmos. Meas. Tech., 6, 1287-1314, doi:10.5194/amt-6-1287-2013.

Peubey, C., A. Benedetti, L. Jones, and J.-J. Morcrette, 2009: GEMS-Aerosol: Comparison and analysis with GlobAEROSOL data. In GlobAEROSOL User Report, October 2009, 11-20.

ECMWF

References: Greenhouse Gases

Agusti-Panareda, A., S.Massart, F.Chevallier,S.Boussetta, G.Balsamo, A.Beljaars, P.Ciais, N.M.Deutscher, R.Engelen, L.Jones and R.Kivi, J.-D.~Paris, V.-H. Peuch, V.Sherlock, A.T.Vermeulen, P.O.Wennberg, D.Wunch, 2014: Forecasting global atmospheric CO2, Atmospheric Chemistry and Physics ,14, 11959-11983, doi:10.5194/acp-14-11959-2014

Chevallier, F., R. J. Engelen, C. Carouge, T. J. Conway, P. Peylin, C. Pickett-Heaps, M. Ramonet, P. J. Rayner, and I. Xueref-Remy, 2009. AIRS-based vs. flask-based estimation of carbon surface fluxes. J. Geophys. Res., 114, D20303, doi:10.1029/2009JD012311.

Chevallier, F., R. J. Engelen, and P. Peylin, 2005. The contribution of AIRS data to the estimation of CO2 sources and sinks. Geophys. Res. Lett., 32, L23801, doi:10.1029/2005GL024229.

Engelen, R.J. and P. Bauer, 2011. The use of variable CO2 in the data assimilation of AIRS and IASI radiances. Q. J. R. Meteor. Soc., doi:10.1002/qj.919

Engelen, R.J., S. Serrar, and F. Chevallier, 2009. Four-dimensional data assimilation of atmospheric CO2 using AIRS observations. J. Geophys. Res., 114, D03303, doi:10.1029/2008JD010739.

Engelen, R.J. and A. P. McNally, 2005. Estimating atmospheric CO2 from advanced infrared satellite radiances within an operational four-dimensional variational (4D-Var) data assimilation system: Results and validation. J. Geophys. Res., 110, D18305, doi:10.1029/2005JD005982

Massart, S. and Agusti-Panareda, A. and Aben, I. and Butz, A. and Chevallier, F. and Crevoisier, C. and Engelen, R. and Frankenberg, C. and Hasekamp, O., 2014: Assimilation of atmospheric methane products in the MACC-II system: from SCIAMACHY to TANSO and IASI0, Atmospheric Chemistry and Physics, 14, 6139–6158,10.5194/acp-14-6139-2014.

ECMWF

References: Fires

Kaiser, J. W., Heil, A., Andreae, M. O., Benedetti, A., Chubarova, N., Jones, L., Morcrette, J.-J., Razinger, M., Schultz, M. G., Suttie, M., and van der Werf, G. R. (2012). Biomass burning emissions estimated with a global fire assimilation system based on observed fire radiative power. Biogeosciences, 9:527–554.

Kaiser, J. W. and van der Werf, G. R. (2012). Global Biomass Burning [in ”State of the Climate in 2011”]. Bull. Amer. Meteor. Soc., 93(7):S54–S55. (also for other years)

Kaiser, J.W., M. Suttie, J. Flemming, J.-J. Morcrette, O. Boucher, and M.G. Schultz, 2009: Global real-time fire emission estimates based on space-borne fire radiative power observations. AIP Conf. Proc., 1100, 645-648.

References: General

Granier, C., Bessagnet, B., Bond, T., D'Angiola, A., Dernier van der Gon, H., Frost, G., Heil, A., Kaiser, J., Kinne, S., Klimont, G., Kloster, S., Lamarque, J.-F., Liousse, C., Masui, T., Meleux, F., Mieville, A., Ohara, T., Raut, J.-C., Riahi, K., Schultz, M., Smith, S., Thompson, A., van Aardenne, J., van der Werf, G., and van Vuuren, D. (2011). Evolution of anthropogenic and biomass burning emissions of air pollutants at global and regional scales during the 1980–2010 period. Climatic Change, 109(1-2):163–190.

Hollingsworth, A., Engelen, R. J., Textor, C., Benedetti, A., Boucher, O., Chevallier, F., Dethof, A., Elbern, H., Eskes, H., Flemming, J., Granier, C., Kaiser, J. W., Morcrette, J.-J., Rayner, P., Peuch, V.-H., Rouil, L., Schultz, M. G., and Simmons, A. J. (2008). Toward a monitor- ing and forecasting system for atmospheric composition: The GEMS project. Bull. Amer. Meteor. Soc., 89(8):1147–1164.