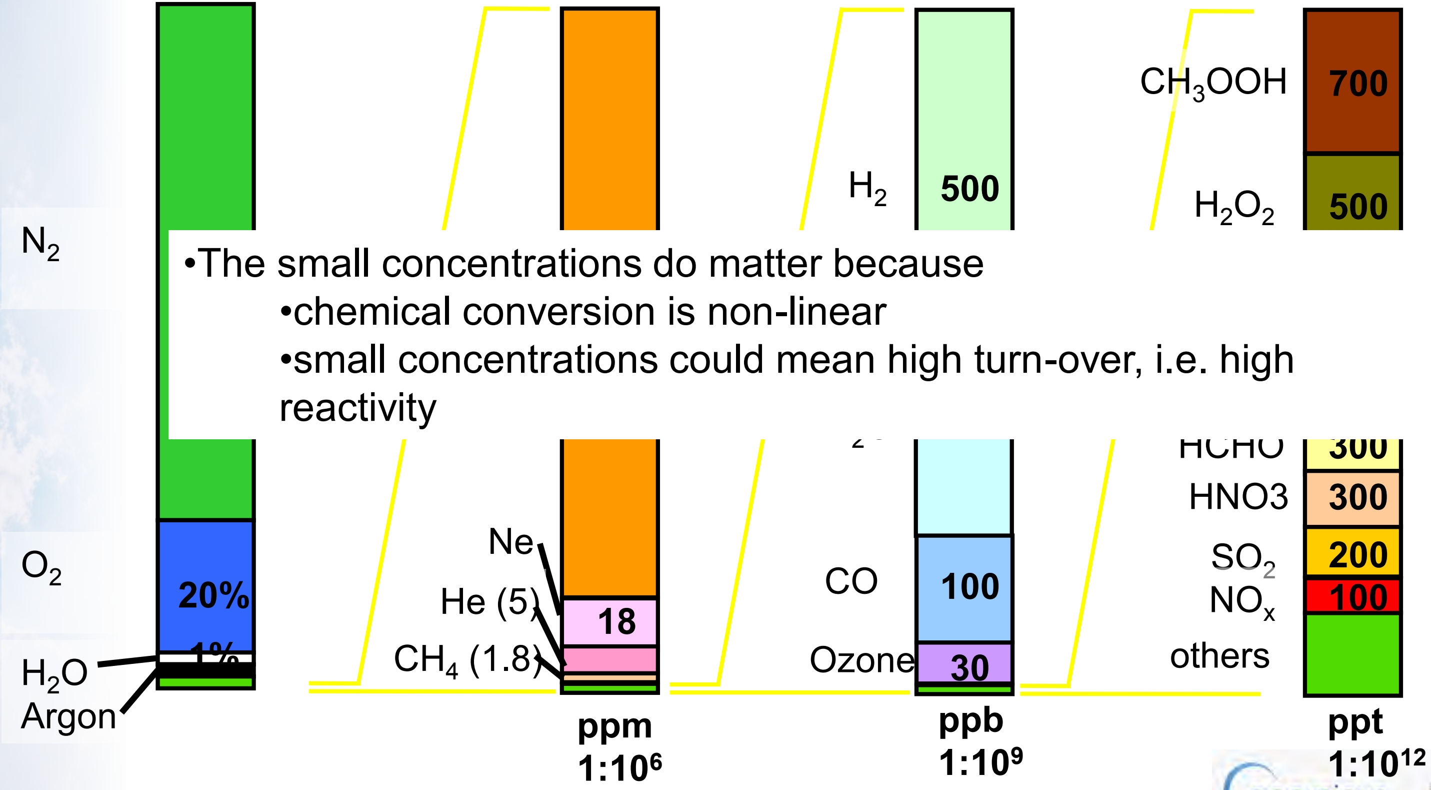
Atmospheric Composition and Numerical Weather Prediction

Johannes Flemming (ECMWF)

Atmospheric Composition – global averages



- The small concentrations do matter because
  - chemical conversion is non-linear
  - small concentrations could mean high turn-over, i.e. high reactivity

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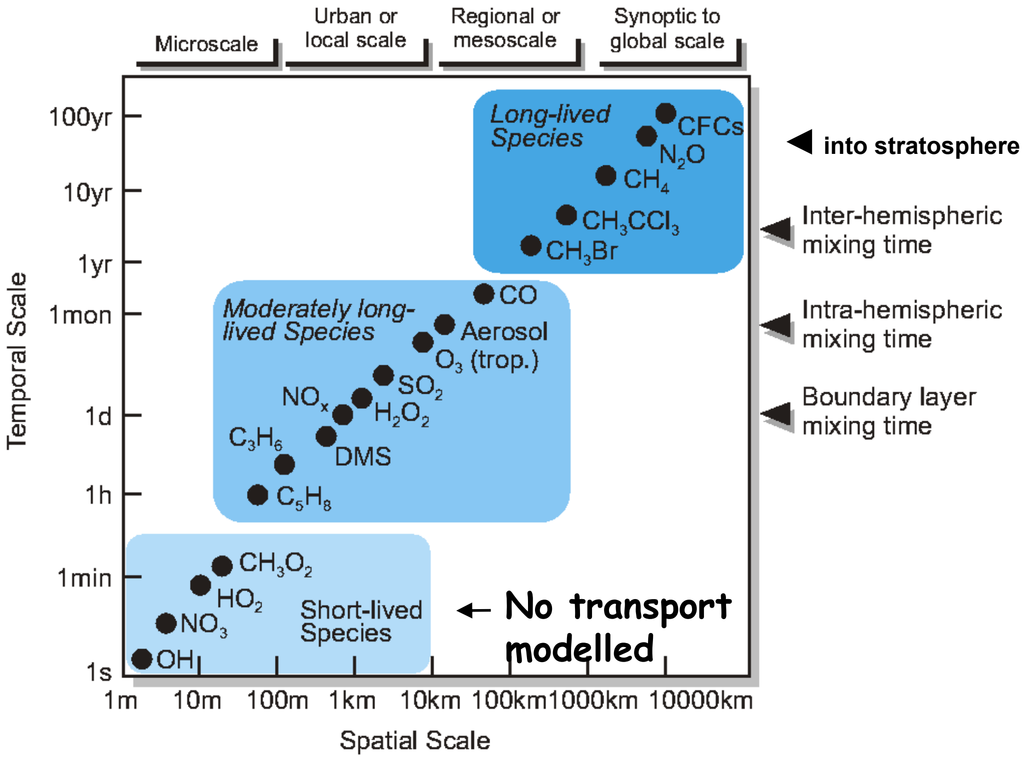
Chemical Lifetime vs. Spatial Scale



After Seinfeld and Pandis [1998]

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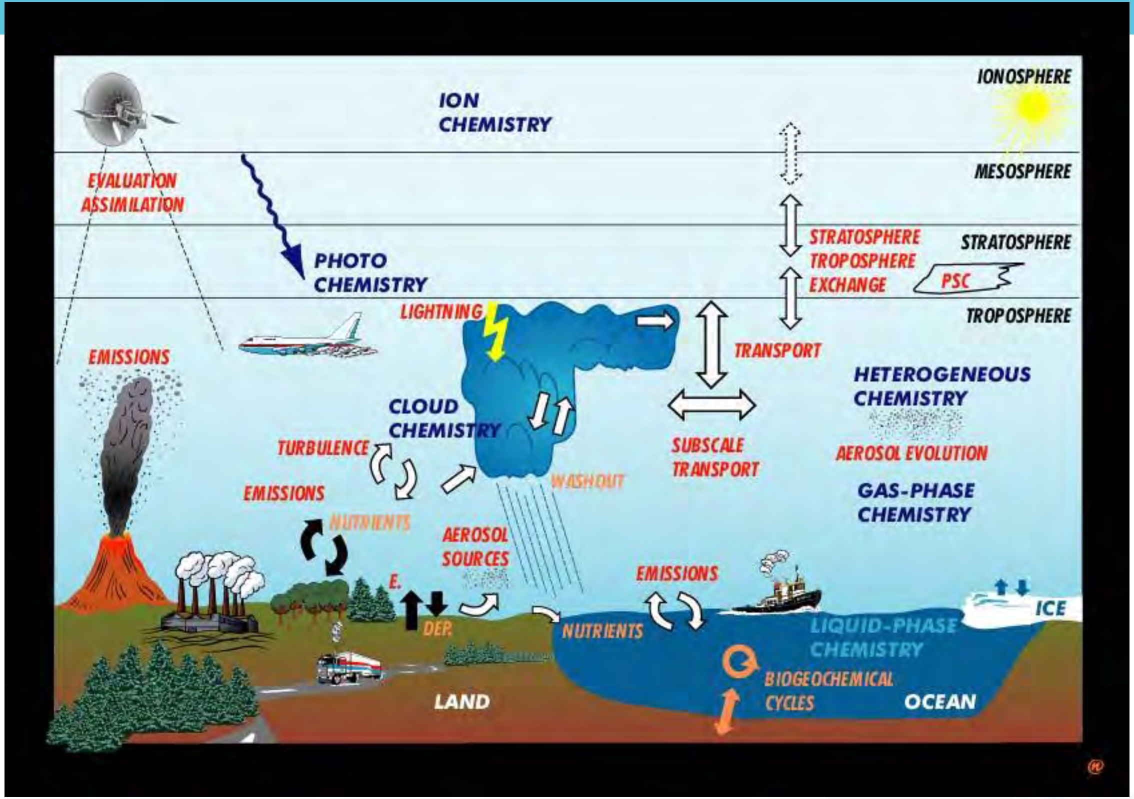
Atmospheric Composition



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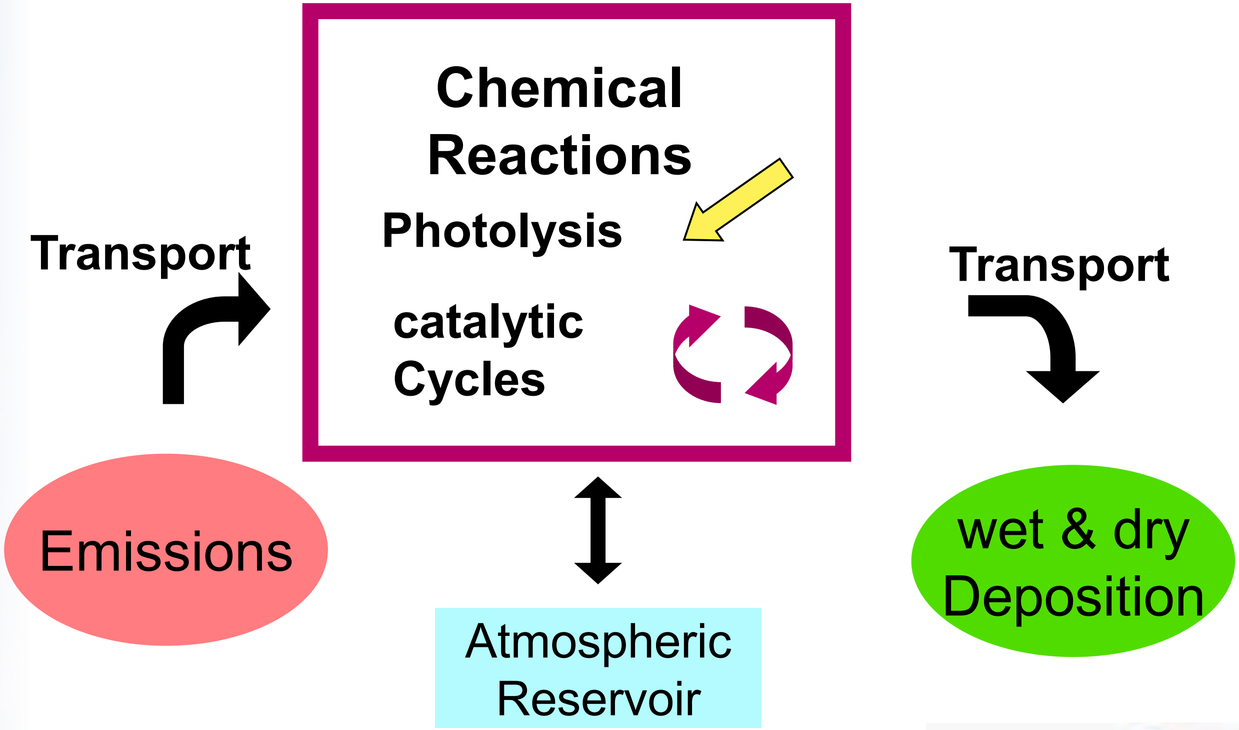
Processes Atmospheric Composition



Modelling of Atmospheric Composition

- Mass balance equation for chemical species (up to 150 in state-of-the-art Chemical Transport Models)

$$\underbrace{\frac{\partial c_i}{\partial t}}_{} + \underbrace{\mathbf{V}_h . \nabla_h c_i + \frac{\partial}{\partial z} w_c c_i - \frac{\partial}{\partial z} K_Z \frac{\partial c_i}{\partial z}}_{\text{Transport}} = \underbrace{E + R - D}_{\text{Source and Sinks}}$$

Transport

Source and Sinks
- not included in NWP

c_i concentration of species i

$E_i \neq f(c_i)$ ... Emission

$R_i = f(c_i, c_j, c_k, c_{m,} ...)$ ... Chemical conversion

$D_i = l_{Dep} c_i$ ... Deposition

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Modelling constituent fluxes in an out of the atmosphere - Emissions

- Surface Emission
  - Anthropogenic activity (from inventories)
  - Biomass burning (observed from satellites)
  - Biogenic and natural (modelled from temperature or wind speed)
  - Dust and Sea Salt emissions based on wind and surface Land
  - Injection modelled with IFS diffusion scheme at surface
- NO lightning emissions
  - Lightning is a major source of Nitrogen Oxide in the atmosphere (about 5 N Tg/y similar to all of Chinas NO_x)
  - 3 parameterisations for flash rate density using cloud height (Price and Rind, 1993) , convective precipitation (Meijer et al, 2001) or updraft velocity & ice cloud height (P. Lopez)

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Flash Rate Parameterizations
1-year average scaled to 40 flashes/s

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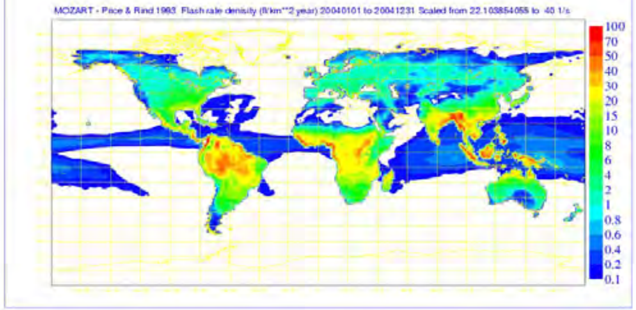
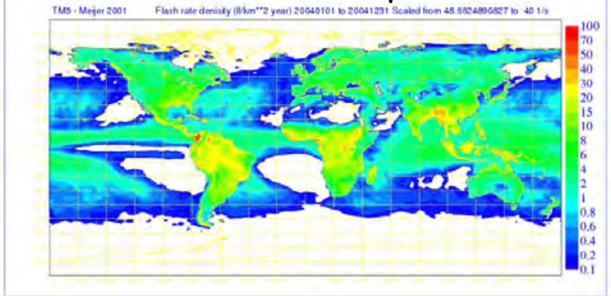
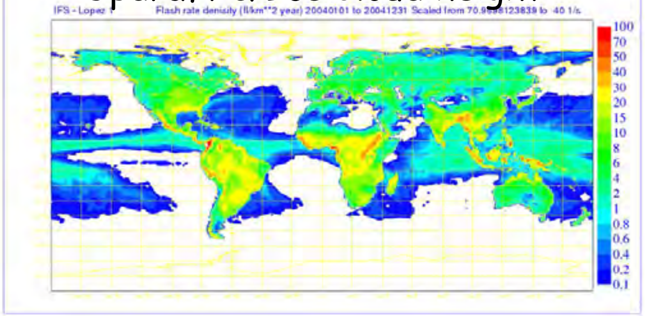
Price and Rind, 1993
Conv. Cloud height



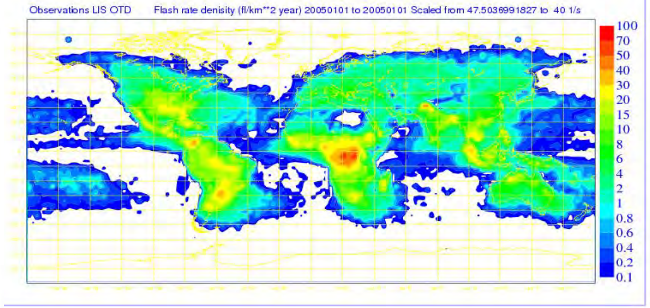
Meijer 2001 (TM5)
Conv. Precip.



Lopez p.c.
Updraft & Ice Cloud height



Observations LIS OTD



Based on a one-year run with C-IFS

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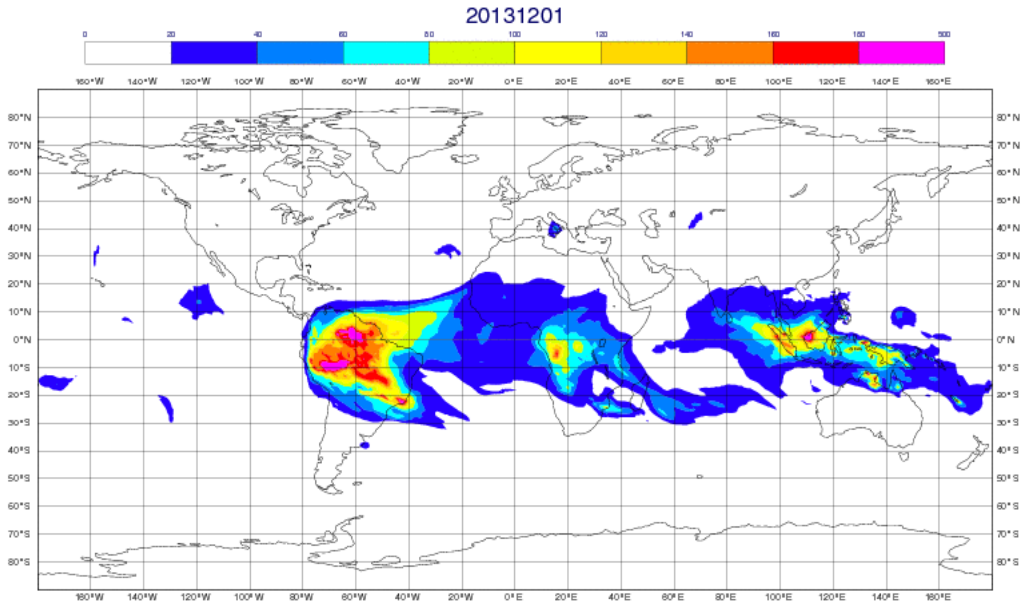
NOx (TC) produced from Lightning

- IFS Lightning parameterisation based on convective precipitation (Meijer et al. 2001)
- LINOx tracer with 5 day lifetime
- Vertical injection profile (“anti C”) Ott et al. 2010



1.12.2013-30.3.2014

used for CAST flight campaign planning

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Global Wildfire Emission Modelling

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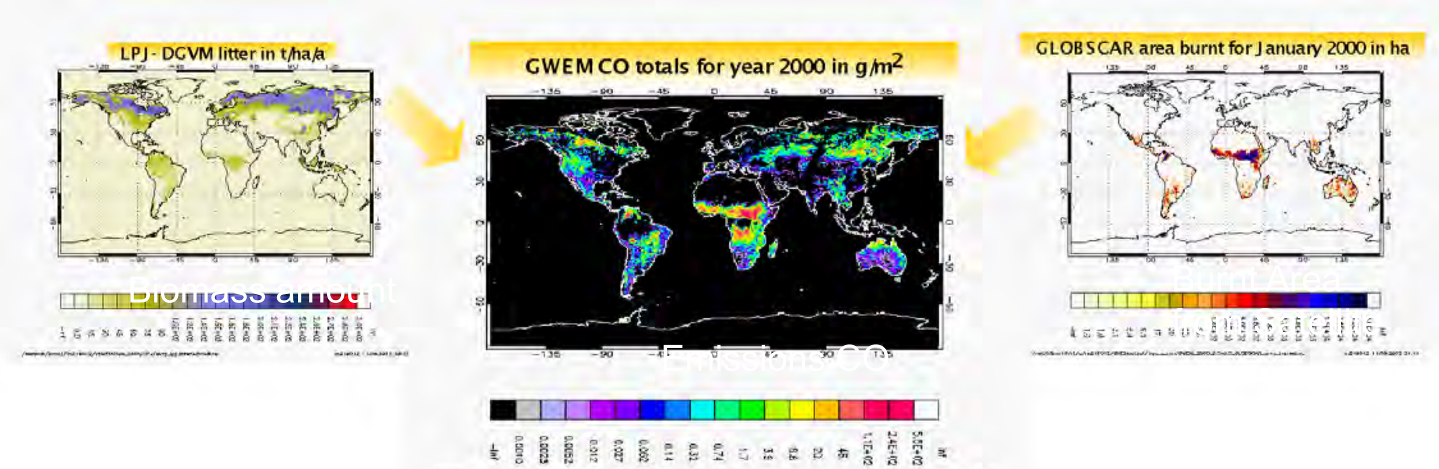
Fire Radiative Power

$$E_i = A \times \beta \times F \times EF_i$$

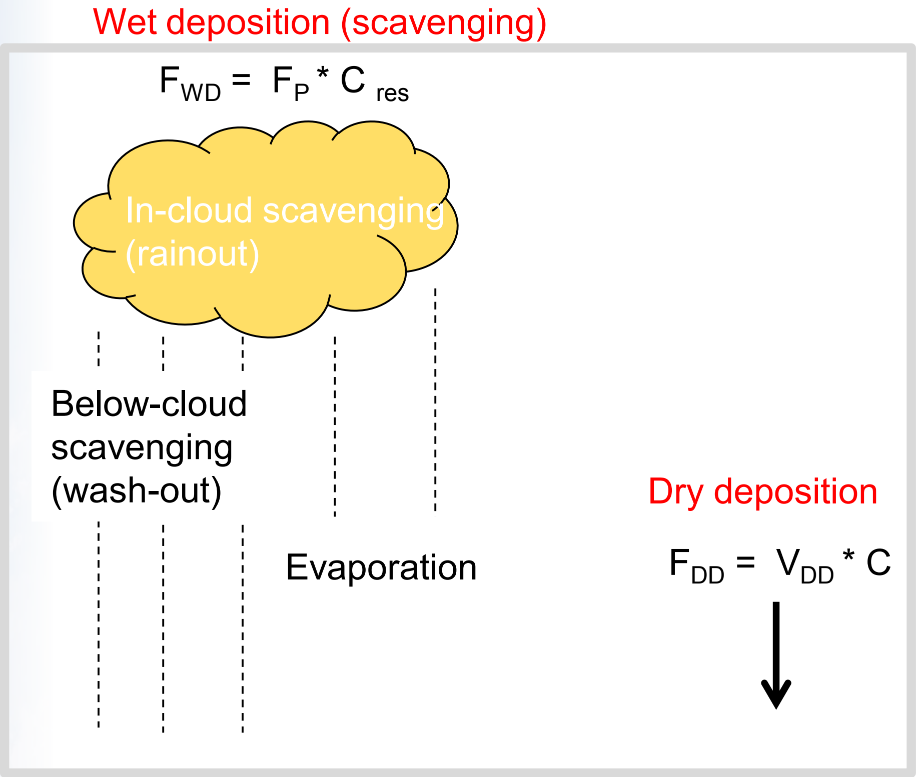
area burnt | combustion efficiency | fuel load | emission factor

1 Method: burnt area satellite retrievals
2 Method: fire radiative power satellite r.

1 BA:GEFD
2 FRP:GFAS, FINN



Deposition Processes



C Concentration
V_{DD} dry deposition velocity
V_{DD} f (Diffusion, surface and canopy)

C_{res} resolved fraction in rain or cloud

C_{res} f (solubility, transfer to droplet)

F_p precipitation flux

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The operational aerosol and chemistry schemes in the IFS (CAMS)

Aerosol (14 species):

AER Bulk scheme

SS_{small}	SS_{mid}	SS_{large}
DU_{small}	DU_{mid}	DU_{large}
OM_{hphob}	OM_{hphil}	
BC_{hphob}	BC_{hphil}	
SO_2	SO_4	
NO_3 fine	NO_3 coarse	NH_4

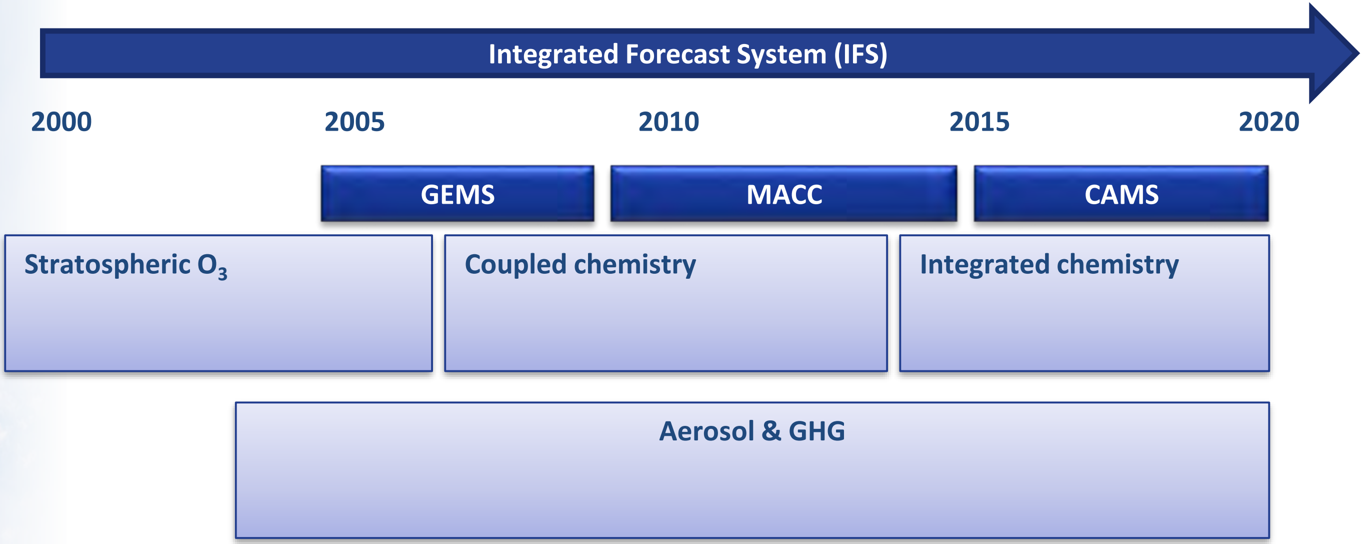
Chemistry (56 species):

CB05 & Cariolle stratospheric ozone scheme

O_3	NO_x	H_2O_2	CH_4	CO	HNO_3
CH_3OOH	CH_2O	PAR	C_2H_4	OLE	ALD_2
PAN	ROOH	ONIT	C_5H_8	SO_2	DMS
NH_3	SO_4	NH_4	MSA	CH_3COCHO	$O_{3\ (strat)}$
Rn	Pb	NO	HO_2	CH_3O_2	OH
NO_2	NO_3	N_2O_5	HO_2NO_2	C_2O_3	ROR
RXPAR	XO_2	XO_2N	NH_2	CH_3OH	HCOOH
MCOOH	C_2H_6	C_2H_5OH	C_3H_8	C_3H_6	$C_{10}H_{16}$
ISPD	NO_3	CH_3COCH_3	ACO_2	$IC_3H_7O_2$	$HYPROPO_2$
NO_xA	PSC				

Atmosphere Monitoring

Development of atmospheric composition in the Integrated Forecast System



GEMS = Global and regional Earth-system (atmosphere) Monitoring using Satellite and in-situ data
MACC = Monitoring Atmospheric Composition and Climate
CAMS = Copernicus Atmosphere Monitoring System

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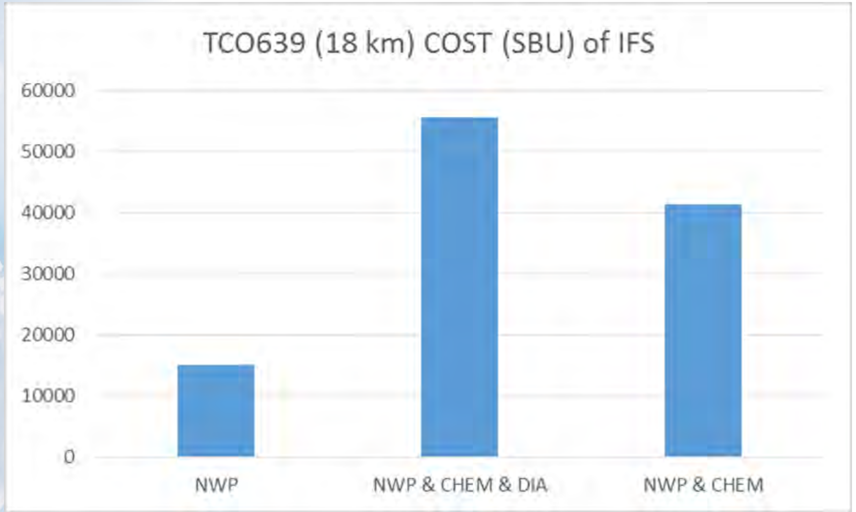
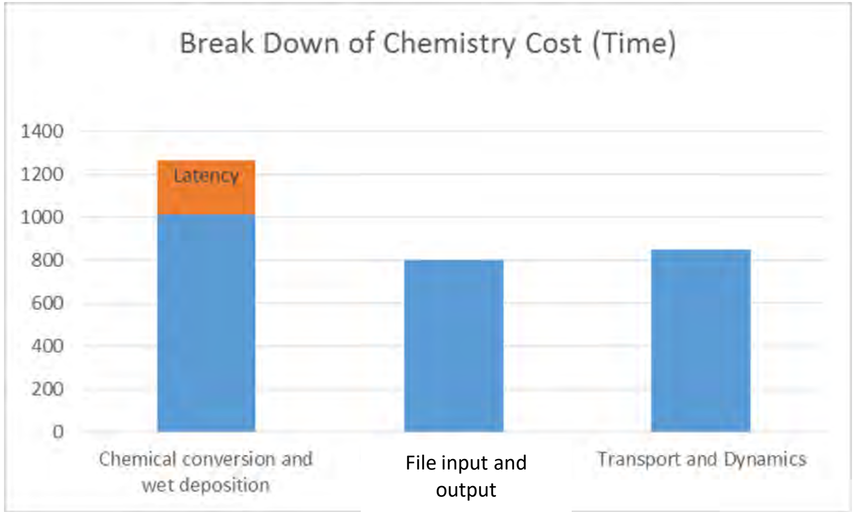
Computational cost of including Atmospheric Composition in IFS





Cost of atmospheric composition in NWP (CB05 + AER)

- Model simulation only : x 4 more expensive
- Data assimilation suite: x 2 more expensive

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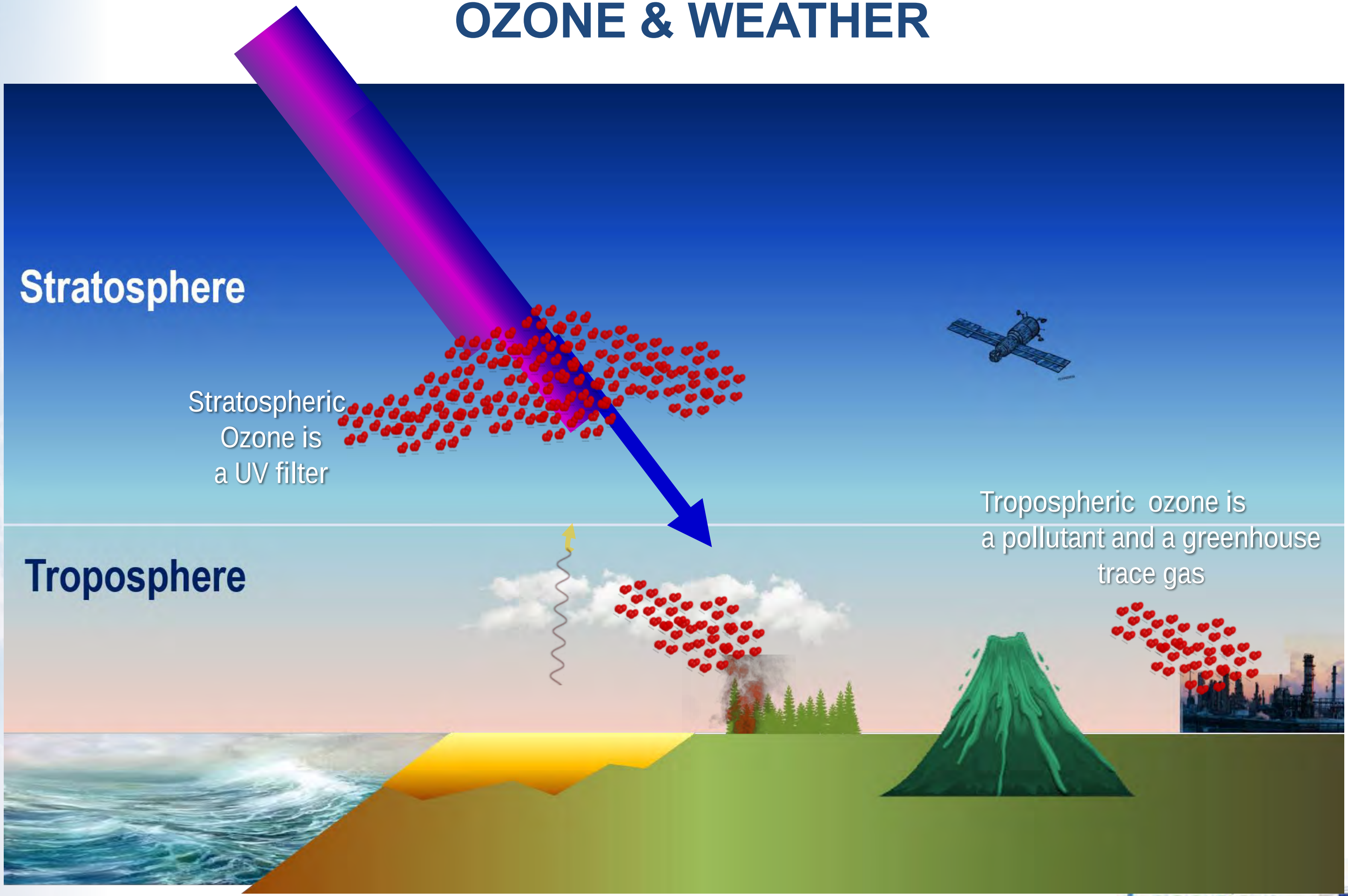
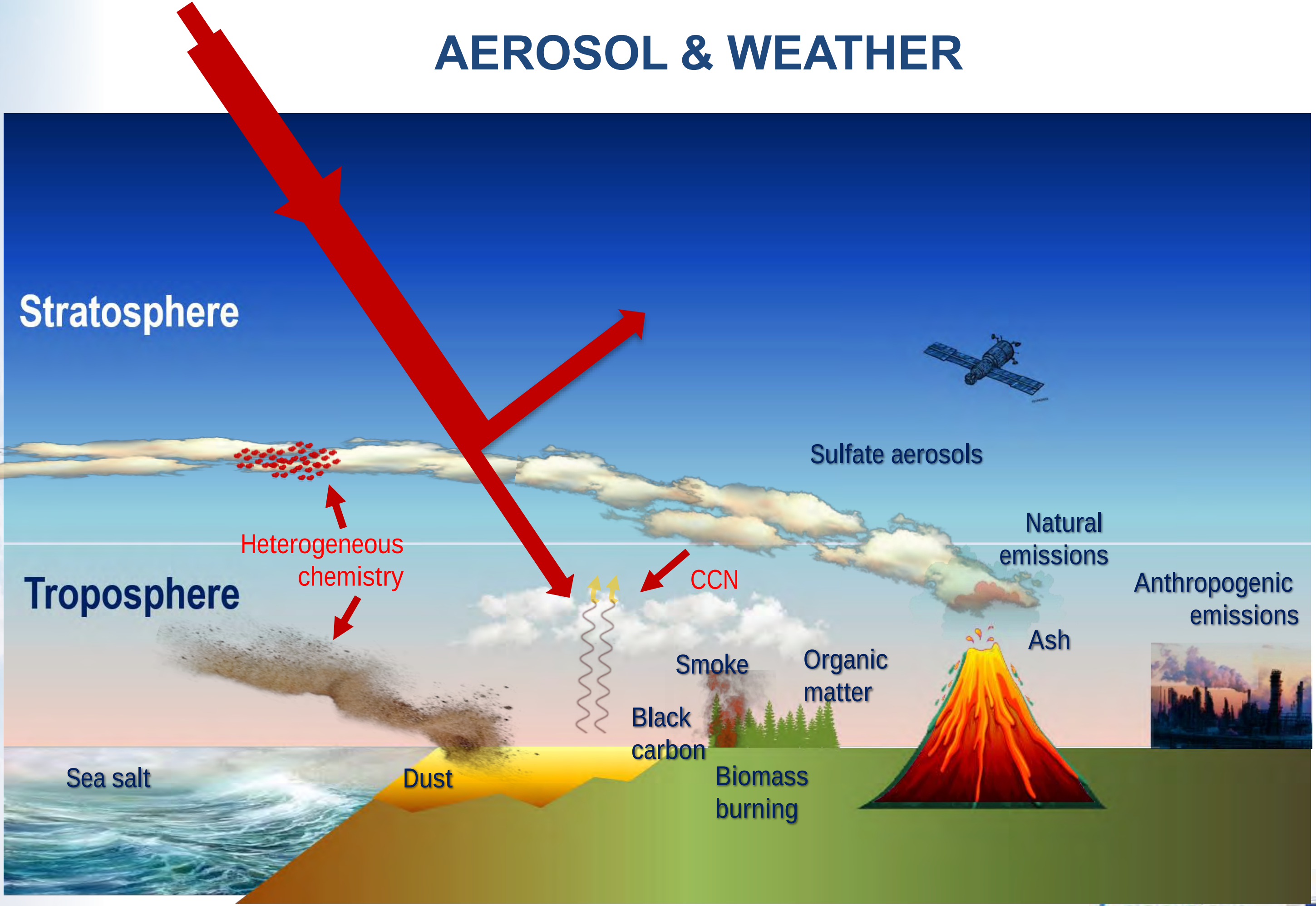
OZONE & WEATHER



AEROSOL & WEATHER



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Aerosol radiative forcing

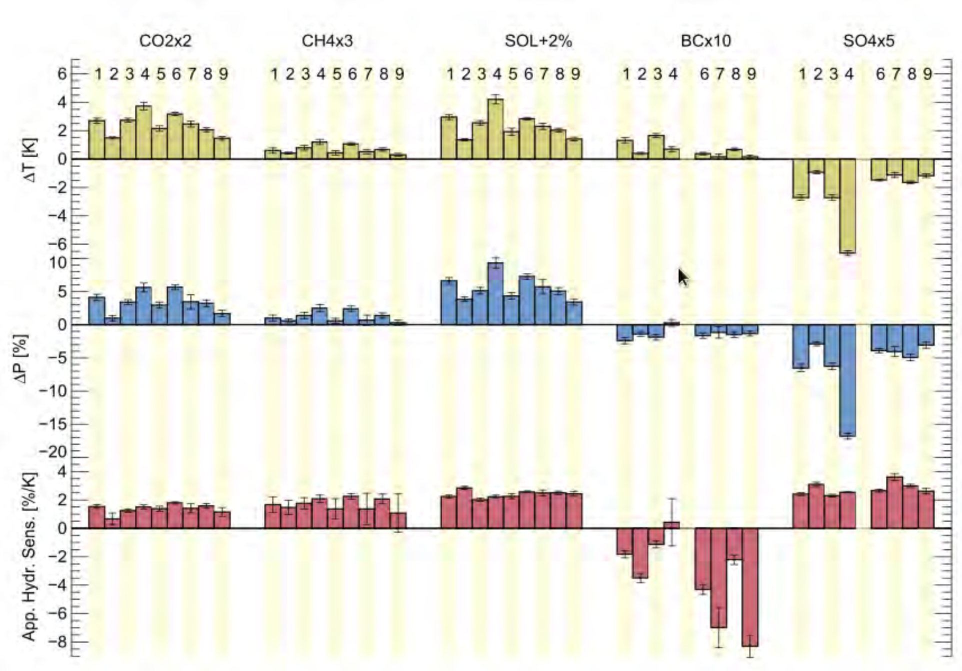

Figure 1 from Samset et al, GRL, 10.1002/2016GL068064, 2016

- Aerosol radiative impacts depend strongly on **what type of aerosols are emitted**
- **Absorbing species** such as black carbon (**BC**) show an **opposite response** in total change in precipitation per degree of global warming (apparent hydrological sensitivity) with respect to the other forcing agents
- A removal of aerosol in a strong Air Quality policy scenario with reduced emissions, can have an **impact on the climate** as aerosols mitigate the induced by greenhouse gases via shortwave cooling.

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Effects of Gases and Aerosols on Meteorology and Climate

- Decrease net downward solar/thermal-IR radiation and photolysis (direct effect)
- Affect PBL meteorology (decrease near-surface air temperature, wind speed, and cloud cover and increase RH and atmospheric stability) (semi-indirect effect)
- Aerosols serve as CCN, reduce drop size and increase drop number, reflectivity, and optical depth of low level clouds (LLC) (the Twomey or first indirect effect)
- Aerosols increase liquid water content, fractional cloudiness, and lifetime of LLC but suppress precipitation (the second indirect effect)

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Atmospheric Composition- Radiation Interactions, Feedbacks and Adujstements

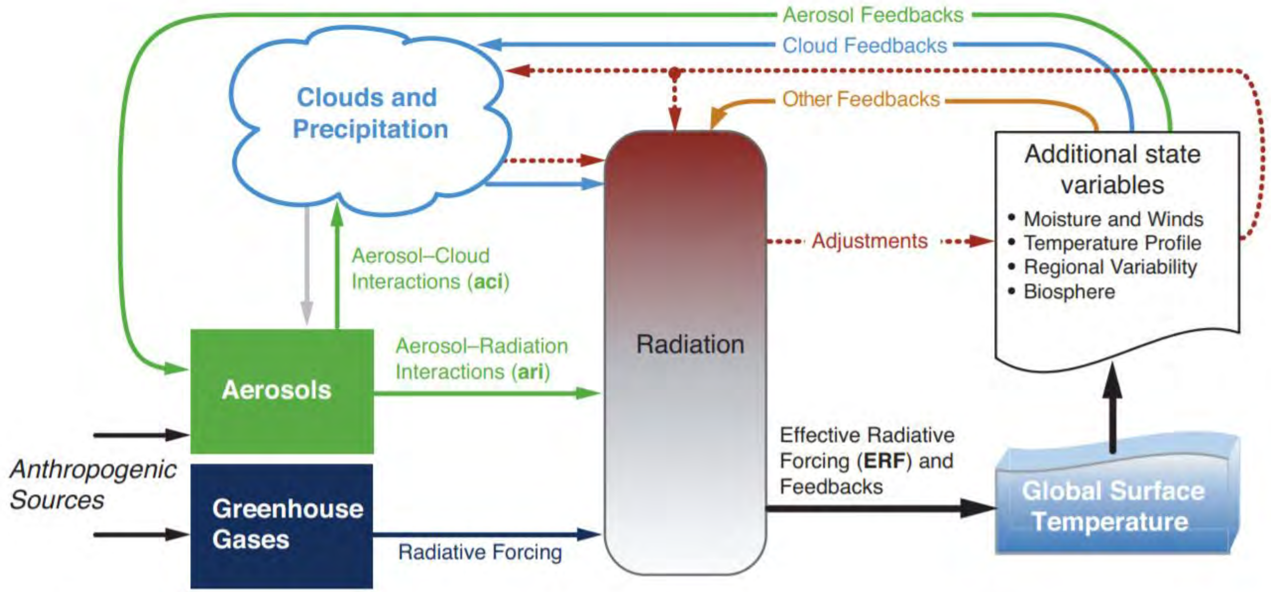
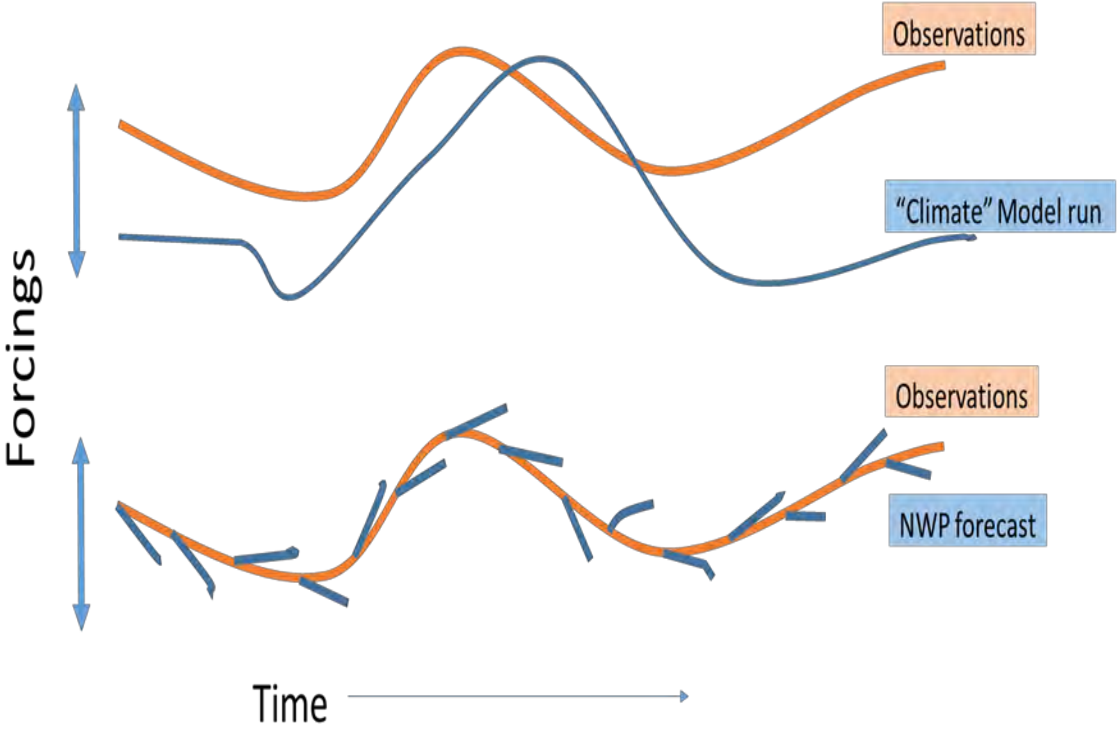


Figure 7.1 | Overview of forcing and feedback pathways involving greenhouse gases, aerosols and clouds. Forcing agents are in the green and dark blue boxes, with forcing mechanisms indicated by the straight green and dark blue arrows. The forcing is modified by rapid adjustments whose pathways are independent of changes in the globally averaged surface temperature and are denoted by brown dashed arrows. Feedback loops, which are ultimately rooted in changes ensuing from changes in the surface temperature, are represented by curving arrows (blue denotes cloud feedbacks; green denotes aerosol feedbacks; and orange denotes other feedback loops such as those involving the lapse rate, water vapour and surface albedo). The final temperature response depends on the effective radiative forcing (ERF) that is felt by the system, that is, after accounting for rapid adjustments, and the feedbacks.

Boucher et al., IPCC 2013

Climate simulation

NWP



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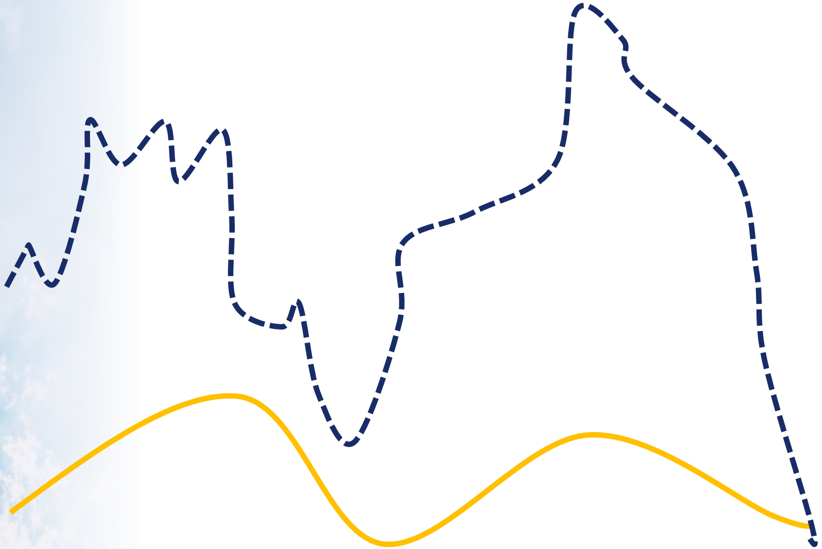
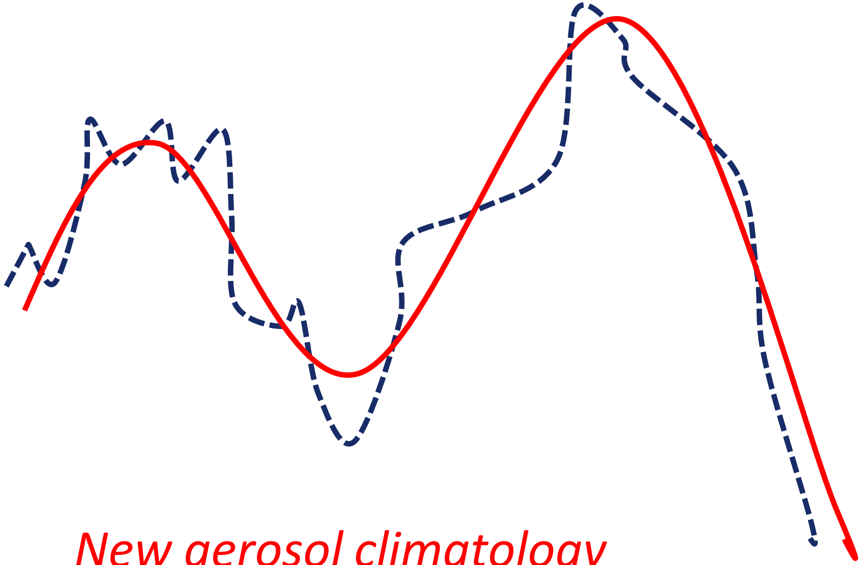


Old aerosol climatology

Prognostic aerosol biased against climatology

= combined mean and variability update



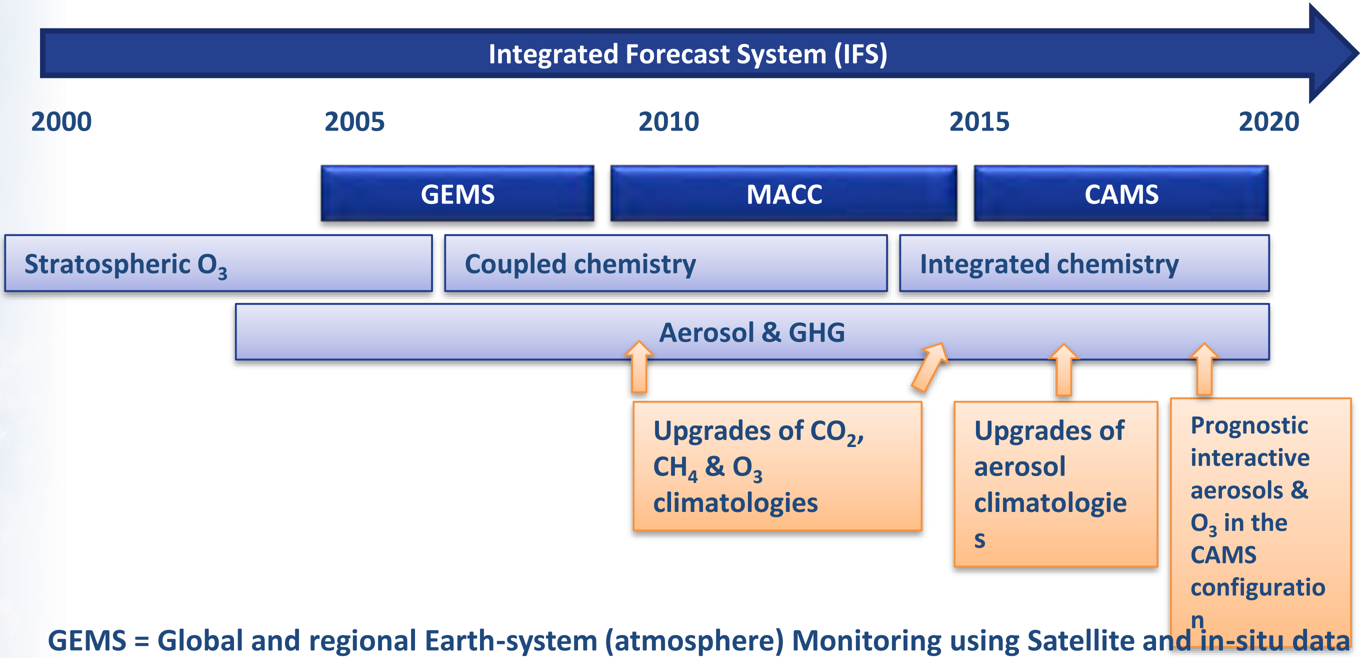
New aerosol climatology

Prognostic aerosol consistent with new climatology

= stepwise mean and variability update

Atmosphere Monitoring

Development of atmospheric composition in the Integrated Forecast System



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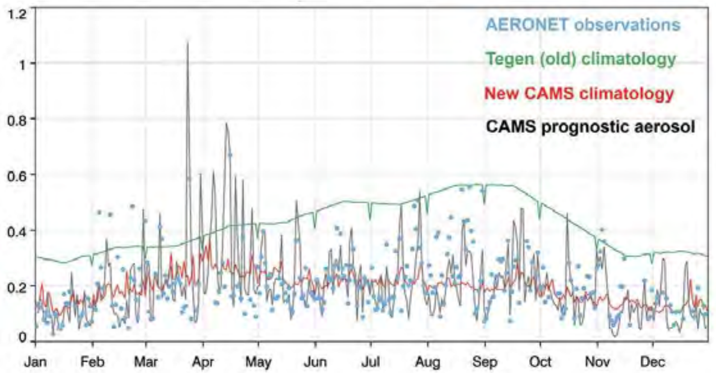
NWP – Weather feedbacks for NWP

- AC development for IFS not mainly driven by AC-NWP feedbacks
- Climatologies account for radiative (direct) effect of aerosol and reactive gases in high-resolution medium-range (10 day) forecasting system
- Upgrade of operational IFS AC climatologies based on CAMS products
- Prognostics aerosol (scattering and absorption) and ozone in radiation scheme in CAMS o-suite (operational)
- Monthly forecasting including aerosol direct effect (still test)
  - Skill introduced by fire emissions not yet possible to forecast
- Seasonal forecasting using prognostic ozone (still test)
  - Progress after updating stratospheric ozone scheme
- AC NWP roadmap document (Dragani et al. 2019 ECMWF TM)
- NWP verification is a challenge
  - all times and areas i.e. high and low AC cases considered
  - uses own analysis

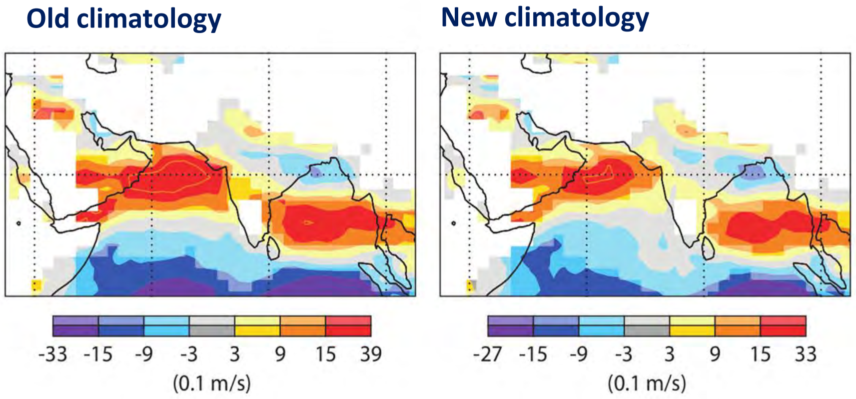
Update of the IFS Aerosol climatology

- **Bozzo et al. (2019, GMDD)** constructed an aerosol climatology from the CAMS interim reanalysis of aerosols (Flemming et al. 2017).
- It has been used operationally since 2016.



A. Bozzo and J. Flemming, ECMWF

Day-5 zonal wind bias at 925 hPa (JJA)



- Better agreement with Aeronet data.
- Reduced bias in the day-5 zonal wind forecasts at 925hPa.
- Higher consistency in IFS between the climatology and the prognostic aerosols.

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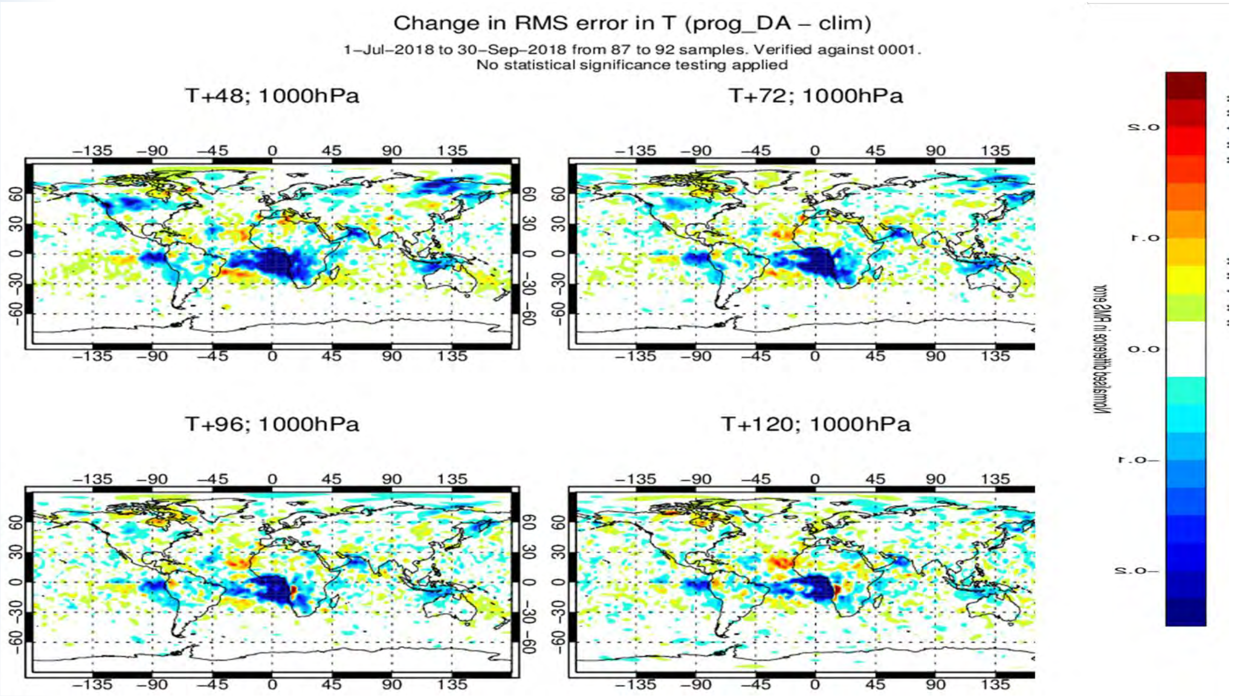
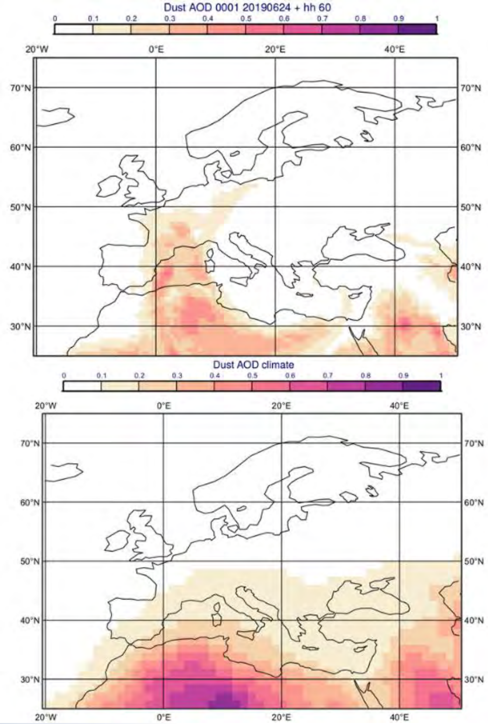
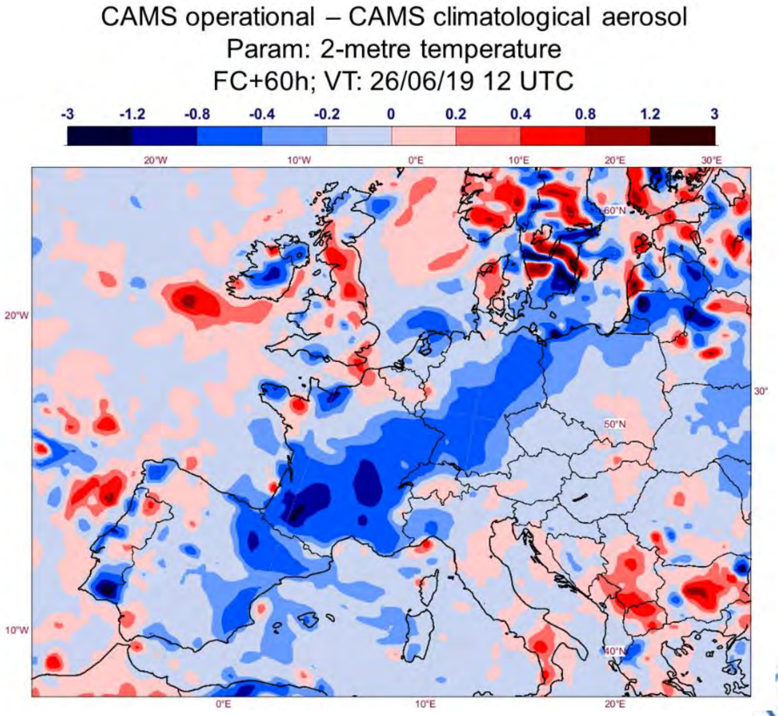
Improvements of NWP verification



Difference in RMSE of temperature at 1000 hPa against analysis between prognostic and climatological aerosol and ozone. Blue areas indicate an improvement with prognostic aerosols and ozone.

Dust Transport Event during Heat Wave in Europe (26.6.2019)





Up to 1 K cooling
Of 2m Temperature because of Dust Transport

60 h Forecast

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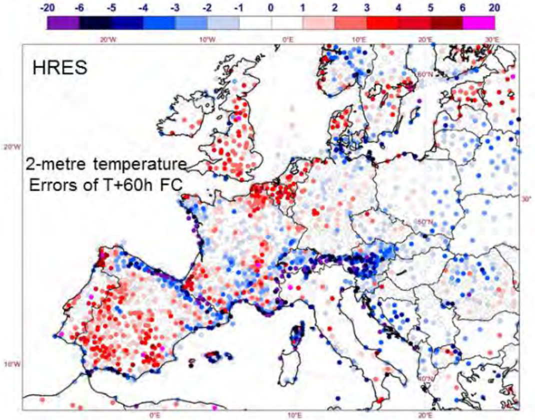
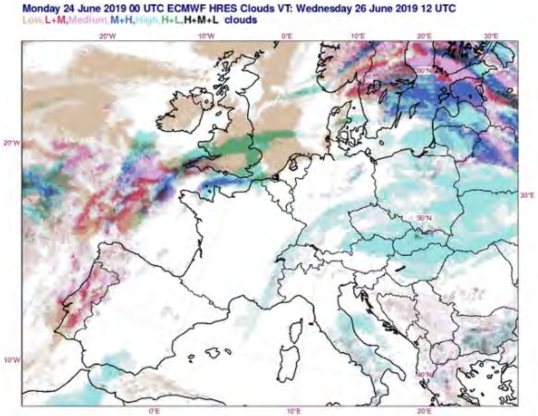
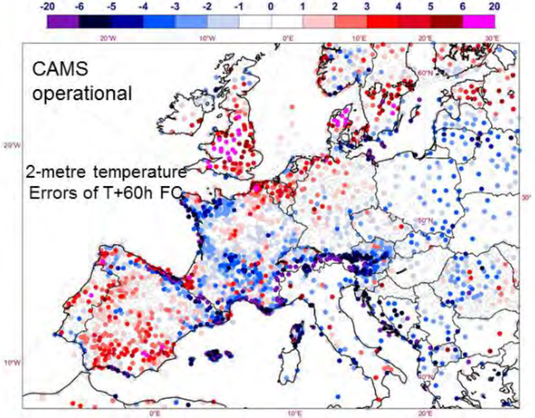
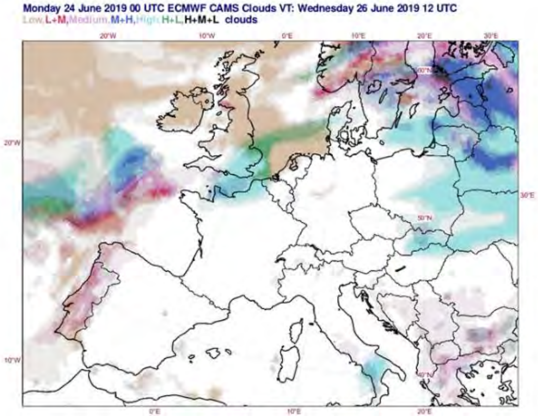
Dust Transport Event during heat wave (26.6.2019)









No improvement by prognostic aerosol compared to climatological aerosol over Central Europe

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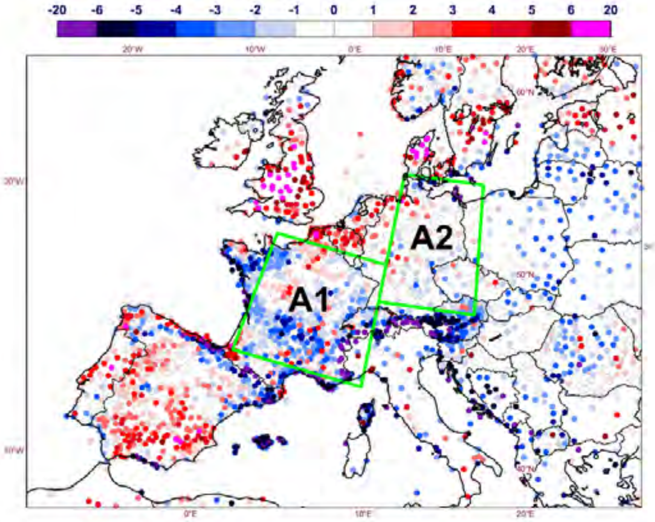
HRES 2m temperature errors



Forecast	Mean error in areas A1&A2
HRES	-0.16 K
CAMS operational	-0.74 K
CAMS with clim. aerosol	-0.25 K

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Aerosol impacts at the S2S scales

- Interactive aerosol simulations use fully prognostic aerosols in the radiation scheme – **only aerosol direct effects are included**
- Free-running aerosols with observed emissions for biomass burning
- Ensemble size is 11 members, T255 (about 60km) resolution, 91 levels
- 5 different start dates around May 1, 55 cases in total
- 6 months simulations

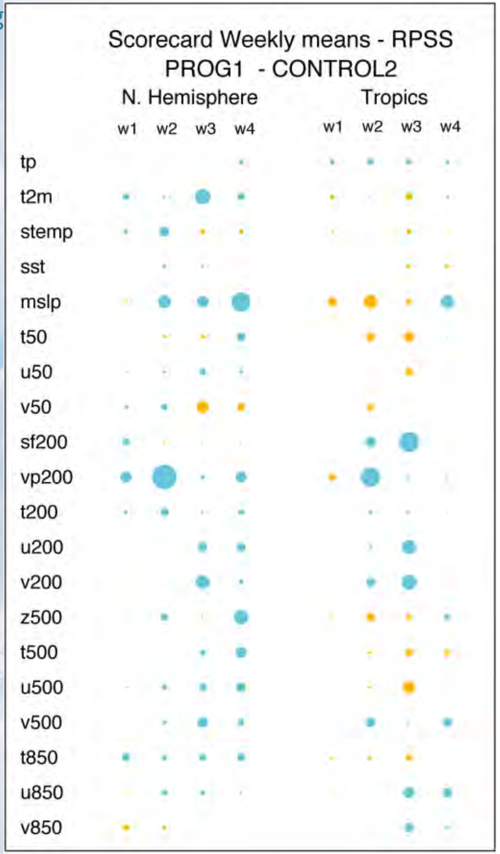
Period 2003-2015

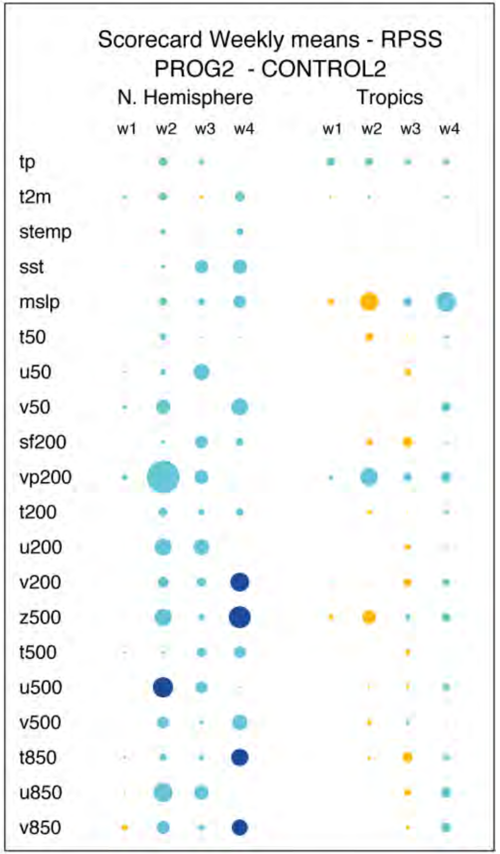
- Results summarized in **Benedetti and Vitart, MWR, 2018**

CONTROL1	Tegen et al (1997) climatology in the radiation
CONTROL2	Bozzo et al (2017) climatology in the radiation
PROG1	Interactive aerosols initialized from the CAMS Interim Reanalysis (Flemming et al 2017)
PROG2	Interactive aerosols initialized from a free-running aerosol simulation

Atmosphere Monitoring

Aerosol impacts on the monthly forecasts: Rank probability skill scores





Interactive aerosol simulations use fully prognostic aerosols in the radiation scheme – **only aerosol direct effects are included**

Observed fire emission applied (GFAS)

Benedetti and Vitart, MWR, 2018

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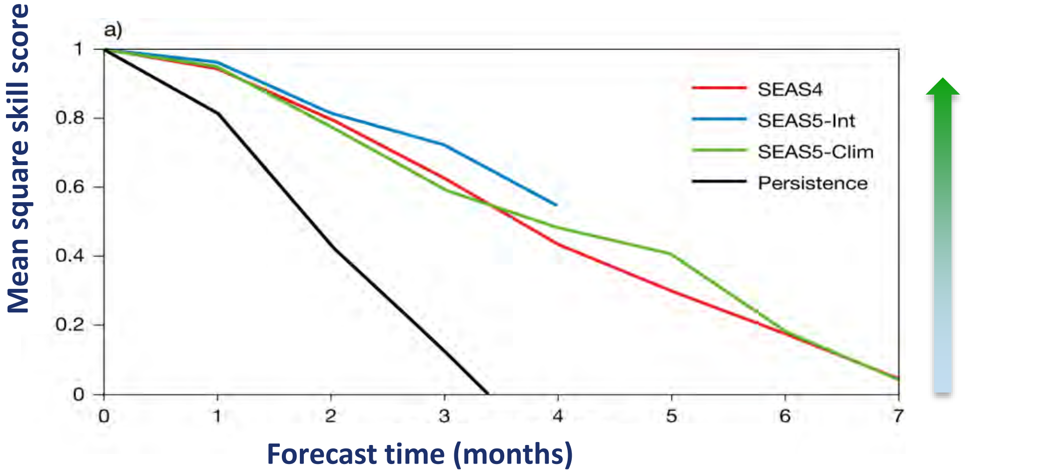
Potential of interactive ozone at seasonal range

Skill scores for the zonal mean temperature forecast

(30hPa, 5ºS-5ºN)

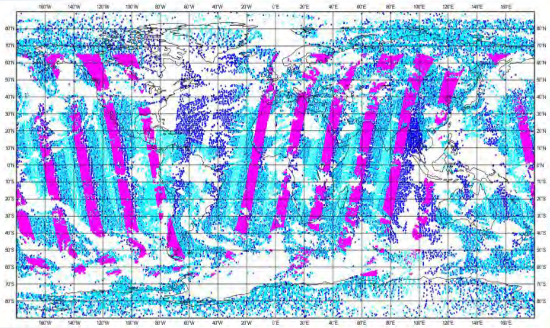


Tim Stockdale, ECMWF

Reactive gases data availability in CAMS NRT system

Atmosphere Monitoring

CO

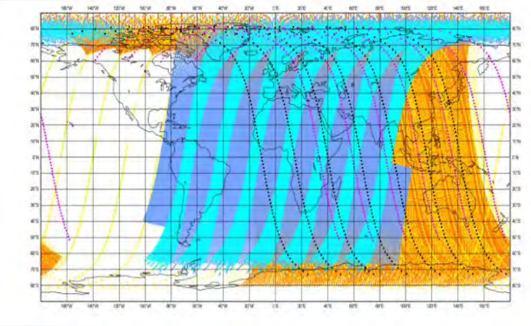


IASI Metop-A

IASI Metop-B

MOPITT TERRA

O3



GOME-2 Metop-A

GOME-2 Metop-B

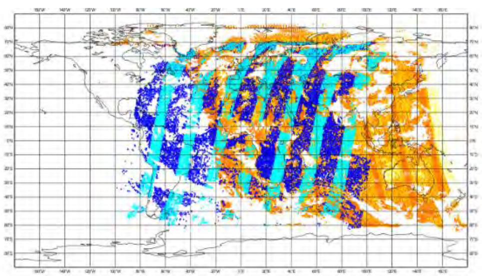
OMI, MLS AURA

SBUV/2 NOAA-19

TROPOMI S5P

OMPS SNPP

Tropospheric NO2



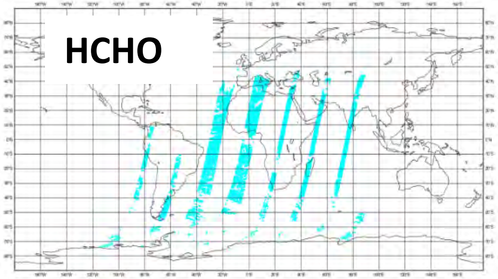
OMI AURA

TROPOMI S5P

GOME-2 Metop-A

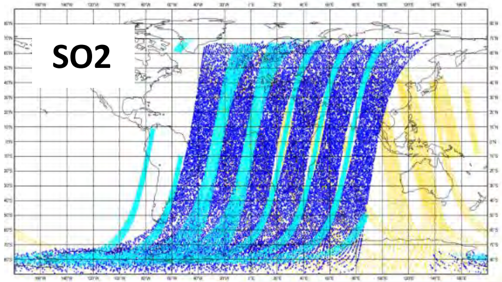
GOME-2 Metop-B

HCHO



GOME-2 Metop-A

SO2



OMI AURA

GOME-2 Metop-A

GOME-2 Metop-B

assimilated

monitored

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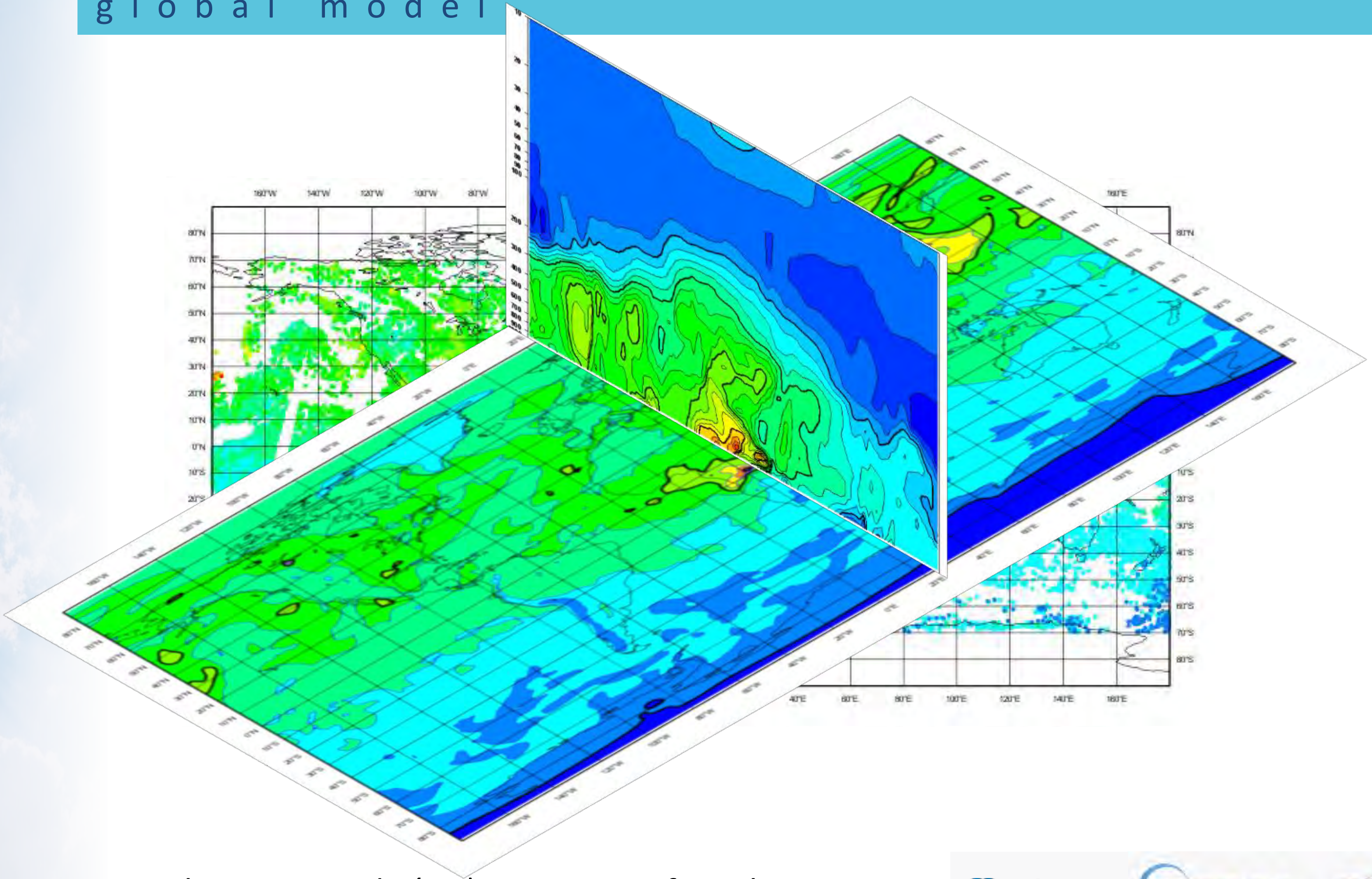
Assimilation of CO observations in a global model



Carbon Monoxide (CO) is a tracer of combustion sources

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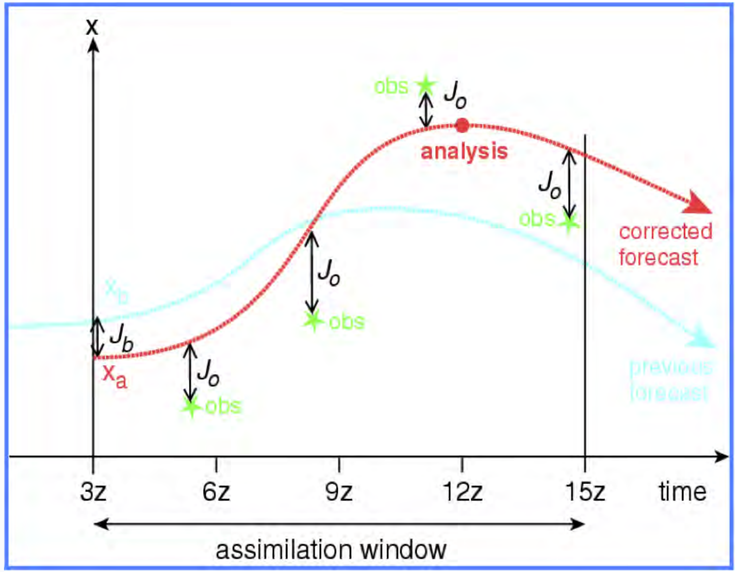
Motivation for combining observations with models

- We need an efficient means of combining the information from ~20,000 observations with a global model at ~40 km horizontal resolution.
- Data assimilation is the process of merging observations with a model in a statistically consistent manner.
- We want to minimize a cost function (J) that evaluates the model background (J_b) and observations (J_o).



$$\mathbf{x}_a = \mathrm{Arg\,min}\,J$$

$$J(\mathbf{x}) = (\mathbf{x}-\mathbf{x}_b)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}_b) + (\mathbf{y}-H[\mathbf{x}])^T\mathbf{R}^{-1}(\mathbf{y}-H[\mathbf{x}])$$

$$= J_b(\mathbf{x}) + J_o(\mathbf{x})$$

forecast, observation, observation operator

$$\mathbf{x}_a = \mathbf{x}_b + \mathbf{A}(\mathbf{y} - \mathbf{H}\mathbf{x}_b)$$

analysis, averaging kernel

Near-real-time satellite data usage

Species	Instruments
Global system	
O_3	**OMI, SBUV, GOME-2, MLS, OMPS S5p**
CO	**IASI, MOPITT, S5p**
NO_2	**OMI, GOME-2, S5p**
SO_2	**OMI, GOME-2, S5p**
Aerosol	**MODIS, PMAp,** VIIRS, S3
CO_2	**GOSAT, OCO-2**
CH_4	**GOSAT, IASI, S5p**
GFAS fire emissions	**MODIS, GOES-E/W*, SEVIRI*,** S3, **VIIRS,** HIMAWARI-8*, GOES-R*

Assimilated **Monitored** Future

*Geostationary platform

A wide-range of atmospheric composition satellite observations are assimilated in the IFS to produce daily analyses.

Control runs (with no data assimilated) and forecasts (initialised from analyses) are also produced in CAMS.

CAMS data used for field campaign planning and evaluating special events.

Composition data additional to thousands of assimilated meteorological data.

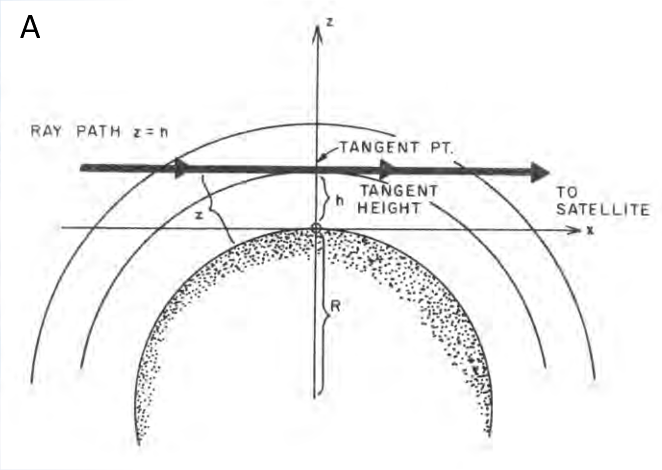
viewing, and (ii) nadir viewing. Limb viewing observes layers of the atmosphere above the horizon and provides good vertical resolution. Nadir viewing looks through the atmosphere directly at the surface and provides good horizontal resolution. As the UTLS is a region with strong vertical gradients (especially in the ozone concentration), the limb viewing geometry is preferred as it can provide the relatively high vertical resolution required.

Satellite viewing geometries

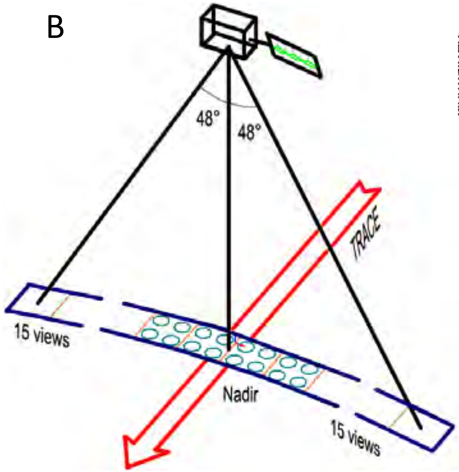
- Using satellite remote sensing to observe vertical profiles of atmospheric consituents is challenging!
- Either:
  - A observe the atmospheric limb in occultation (using Sun, Moon, stars) or thermal emission – limb geometry
  - B use spectral information/scattering to extract information from specific layers in the atmosphere – nadir geometry

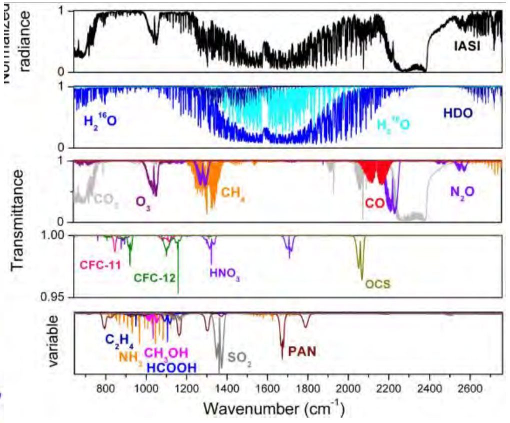
2.1 Satellite Limb Sounding

A



B





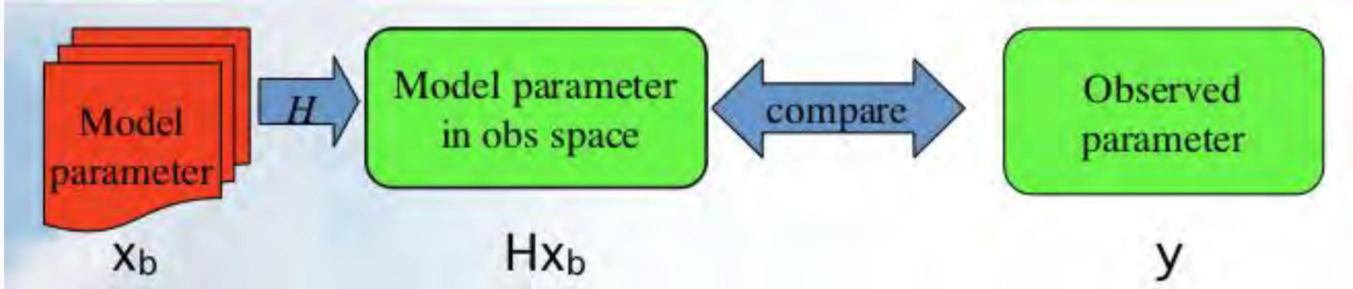
Example of IASI taken from Clerbaux et al., ACP, 2009

Figure 2.1: Satellite limb viewing geometry (NASA, 1978)

Atmosphere Monitoring

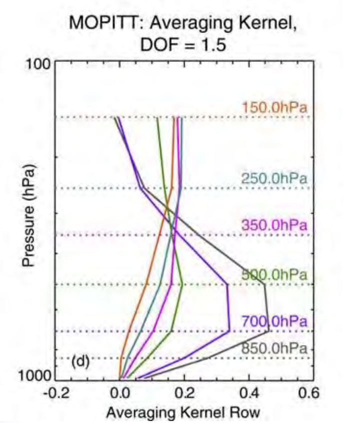
Two of the ways in which limb viewing geometries can be used to make at-

Observation operator

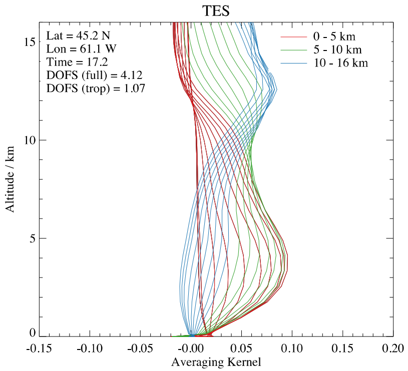


- To assimilate any data we need a means of directly comparing the model parameter with an observed quantity.
- The observation operator (H) converts a model parameter for comparison against an observation in observation space (i.e., taking into account location, time of day, etc.).
- Simplest form is interpolation from model grid to observation location (e.g., in situ measurements).
  - It could also include complex transformations based on the physics of the measurement.

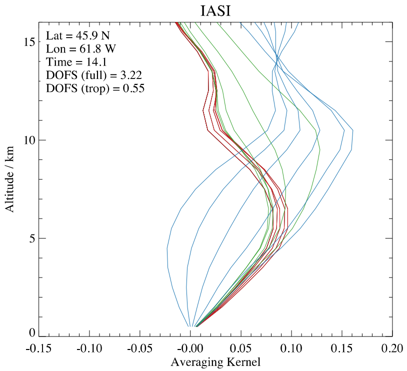
- Averaging kernels provide the information required to directly compare satellite retrievals with models/in situ observations.



MOPITT CO



TES O_3



IASI O_3

- Data assimilation into NWP models redistributes atmospheric composition observations to provide vertical information.
  - Validation against independent data is essential!

{Product Level Choice Atmospheric Composition

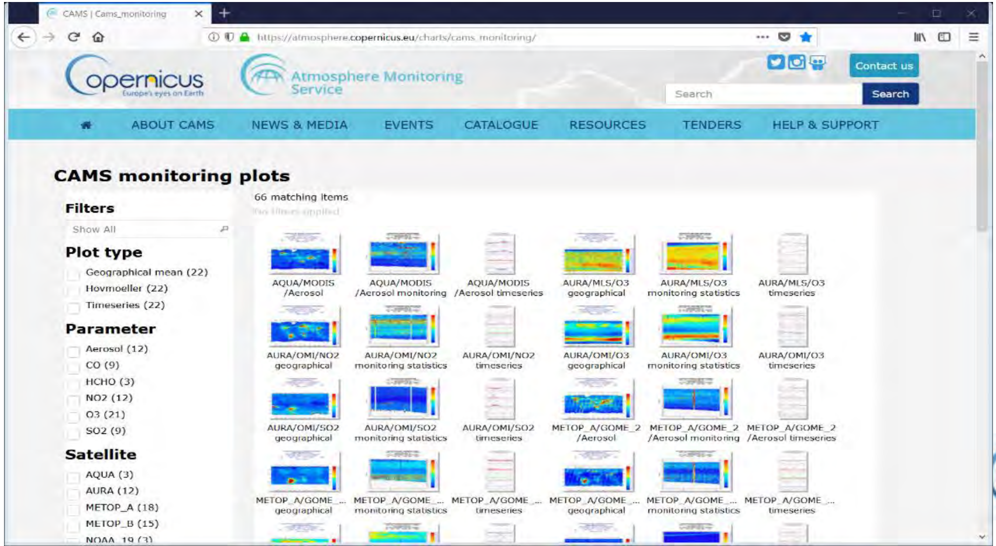
What is pragmatic and accurate?

- Fully specified profile retrieval with all needed information
- Column retrieval with averaging kernel
- Radiance assimilation with fast approximate RT model
- Radiance assimilation with very accurate RT model

Atmosphere Monitoring

Summary

- TROPOMI/Sentinel-5P are monitored by CAMS
- O3 data have been operationally assimilated since Dec 2018
- Assimilation tests with NO2, CO and SO2 are under way
- Monitoring plots on: atmosphere.copernicus.eu/charts/cams_monitoring/



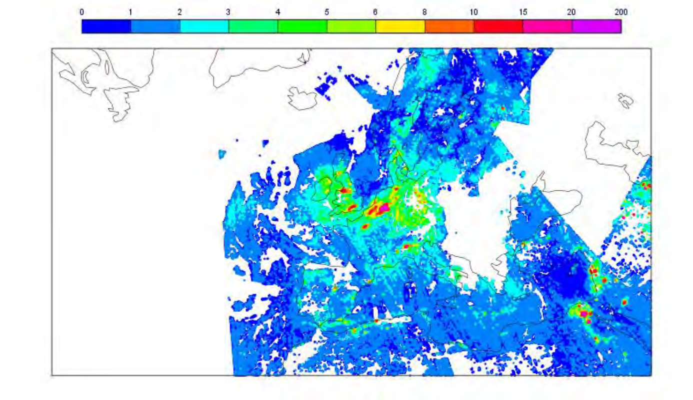
European Commission

Atmosphere Monitoring

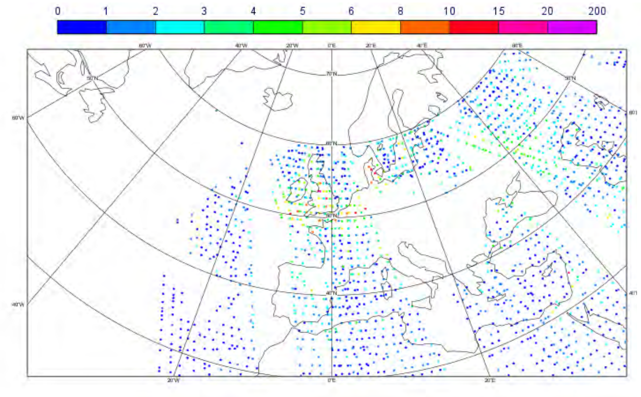
New data: Tropomi (S5P) data coverage

27 June 2018

TROPOMI (ESA, full resolution)

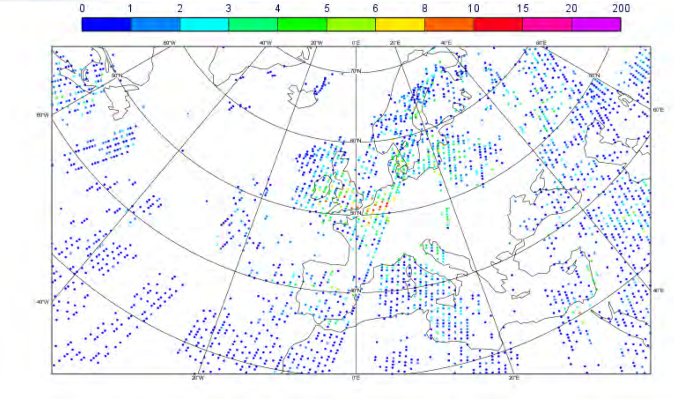


OMI (DOMINO-V2)

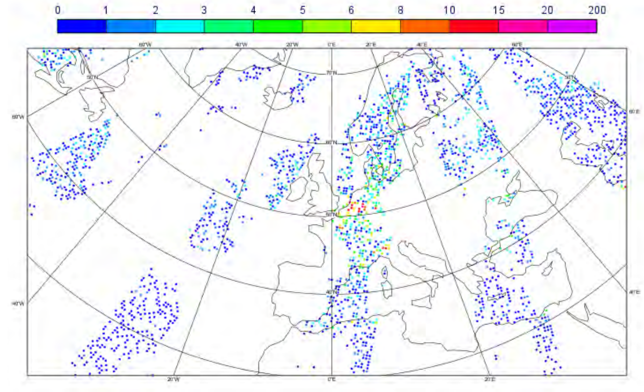


- GOME-2 and OMI thinned to 0.5° x 0.5° and cloud cleared
- TROPOMI cloud cleared

GOME-2B (GDP v4.8)



GOME-2A (GDP v4.8)

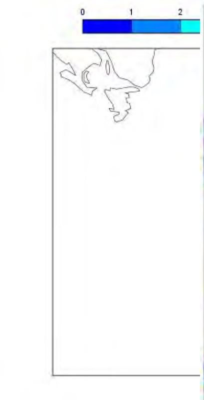


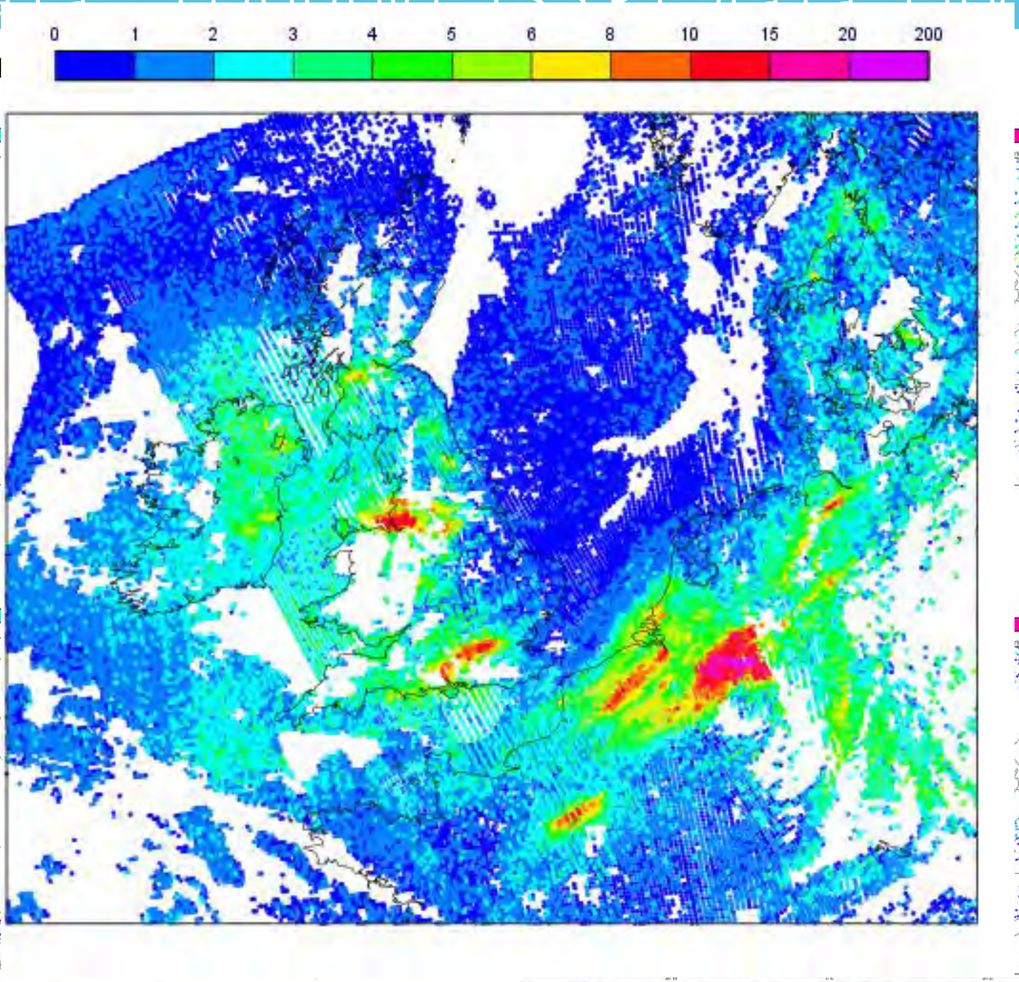
European Commission

Atmosphere Monitoring

New data: Tropomi (S5P) data coverage

TR



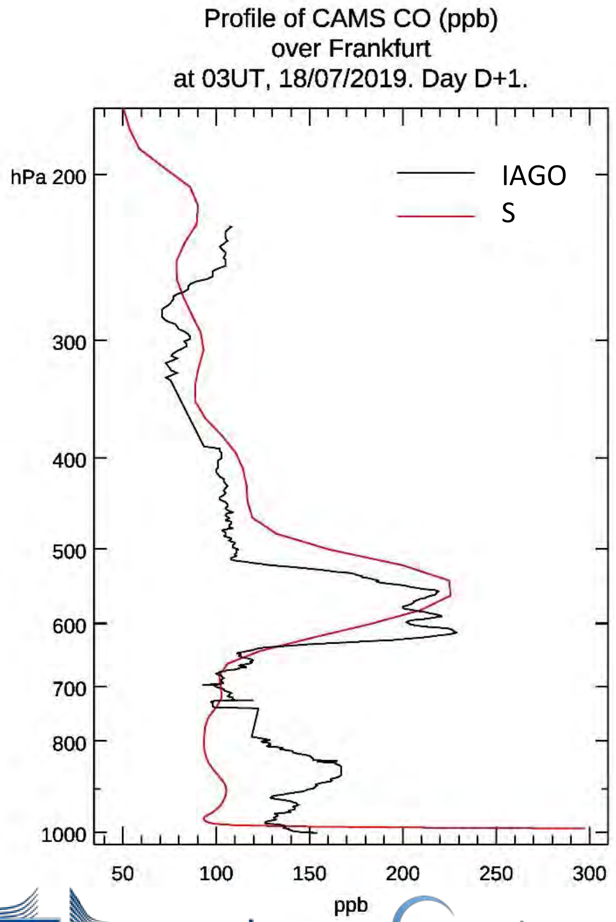


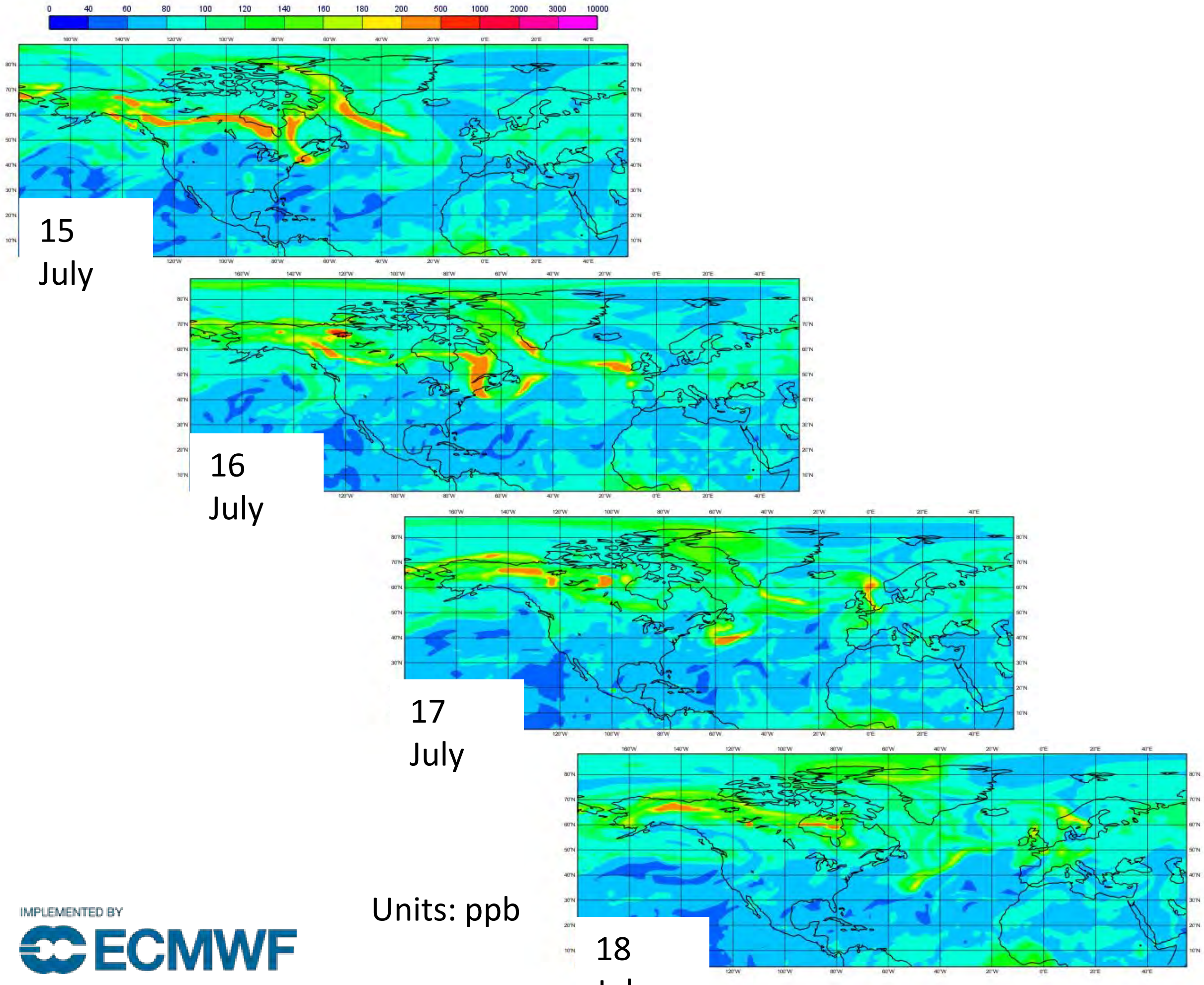
GOM

27 June 2018

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

CO transport form North American fires in July 2019





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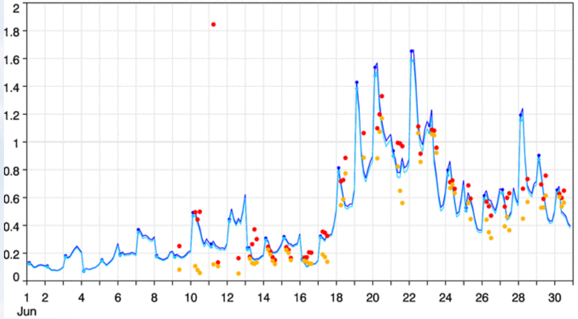
Atmosphere Monitoring

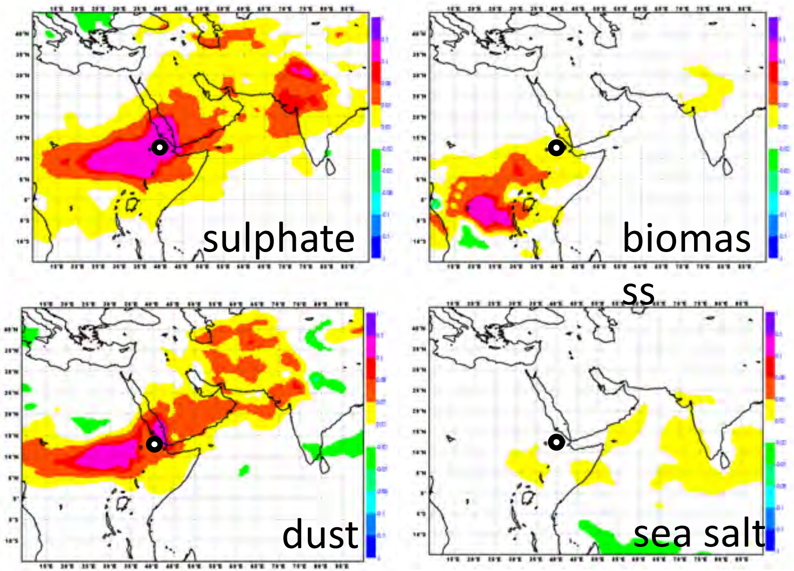
Example for wrong aerosol attribution

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



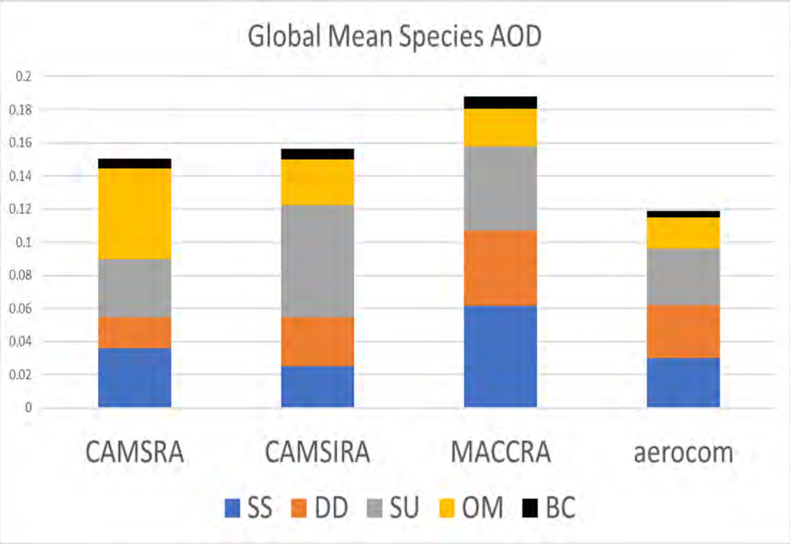
MACC AOD analysis
AERONET total AOD
AERONET fine mode AOD



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

Aerosol Speciation in Data assimilation



Global aerosol speciation (AOD) of CAMS, CAMS-interim and the MACC-RA and the median of the AEROCOM model (Kinne et al. 2006)