Chemistry data assimilation validation with respect to independent data

Angela Benedetti

with contributions from:

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Outline

- Overview of GEMS/MACC projects
- Validation metrics
- Greenhouse gases analysis & validation
- Aerosol analysis & validation
- Reactive gases analysis & validation
- Summary & items for discussion

GMES

Global Monitoring for Environment and Security

- a European initiative for the provision of information services on environment and security, led by the EC and ESA

- fostering the development of five core services: Atmosphere, Land, Ocean, Emergency Response and Security

GEMS

Global and regional Earth-system Monitoring using Satellite and in-situ data

- a 32-partner EC project developing systems for the core GMES atmospheric service

MACC

Monitoring Atmospheric Composition and Climate

- A 48-partner merger of GEMS and ESA-funded PROMOTE

GEMS subprojects

GHG: greenhouse gases modelling, validation and flux inversion

GRG: reactive gases modelling, coupling between Chemical Transport Models and the ECMWF Integrated Forecasting System, validation

AER*:* incorporation of an aerosol scheme in the ECMWF model, validation

RAQ: production of regional forecasts of chemical species and air quality indices based on an ensemble of air-quality models on the European scale.

PRO: 4D-Var analysis of greenhouse gases, reactive gases and aerosol using developments from GHG, GRG, and AER. Provision of daily analyses and forecasts, and retrospective analyses for the years 2003-2007.

VAL: cross-theme validation of the integrated GEMS system.

GEMS tasks at ECMWF

- **Coordinate project** *(Adrian Simmons)*

- **Extend IFS model to includes aerosols, carbon dioxide and methane** *(Johannes Kaiser, Jean-Jacques Morcrette, Soumia Serrar)*

- **Add faster reactive species to IFS and couple with external models for chemical tendencies** *(Johannes Flemming)*

- **Develop data assimilation for new species** *(Angela Benedetti, Antje Inness, Richard Engelen)*

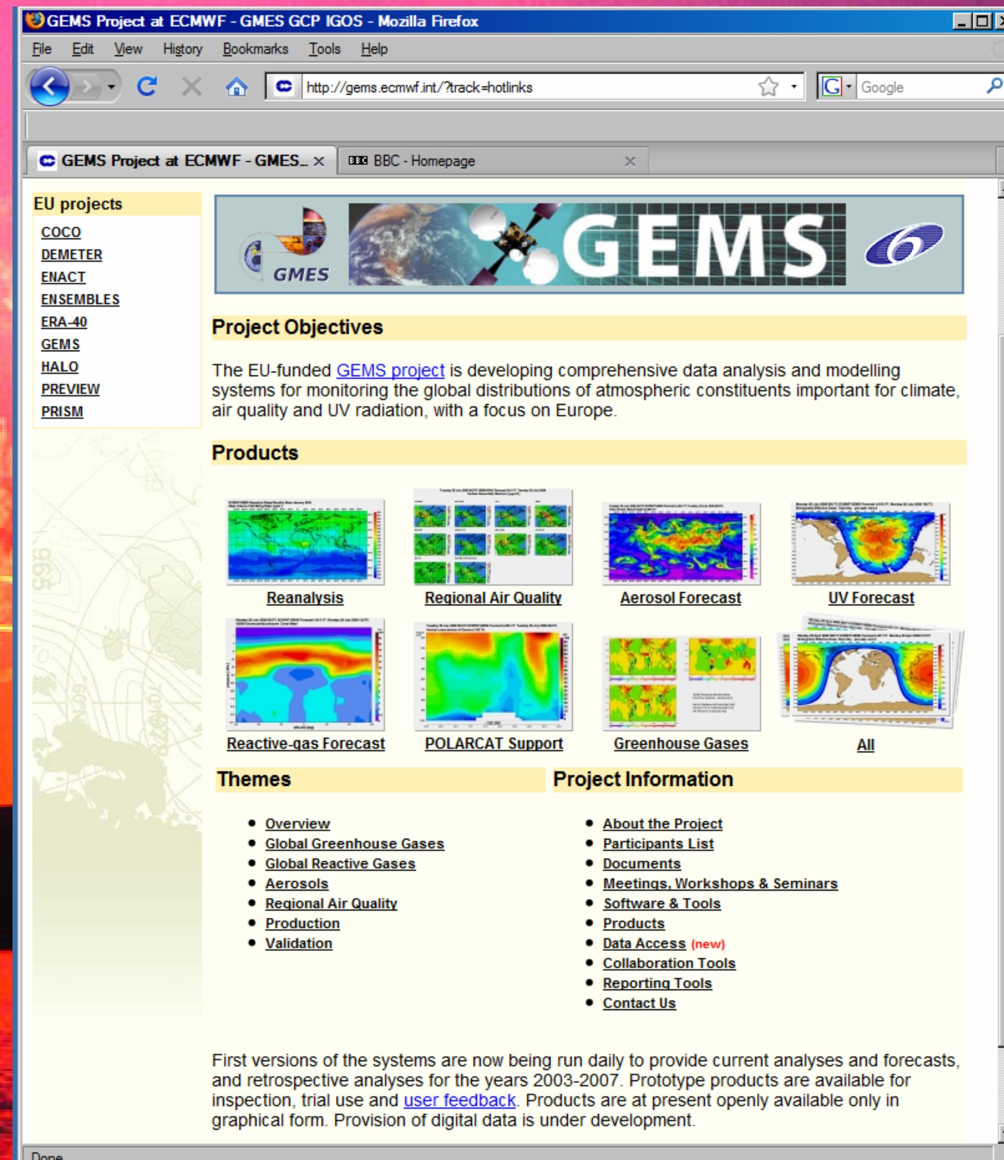
- **Acquire global data, develop validation and support regional air-quality forecasting** *(Luke Jones, Miha Razinger, Martin Suttie)*

- **Provide prototype production systems** *(Everyone)*

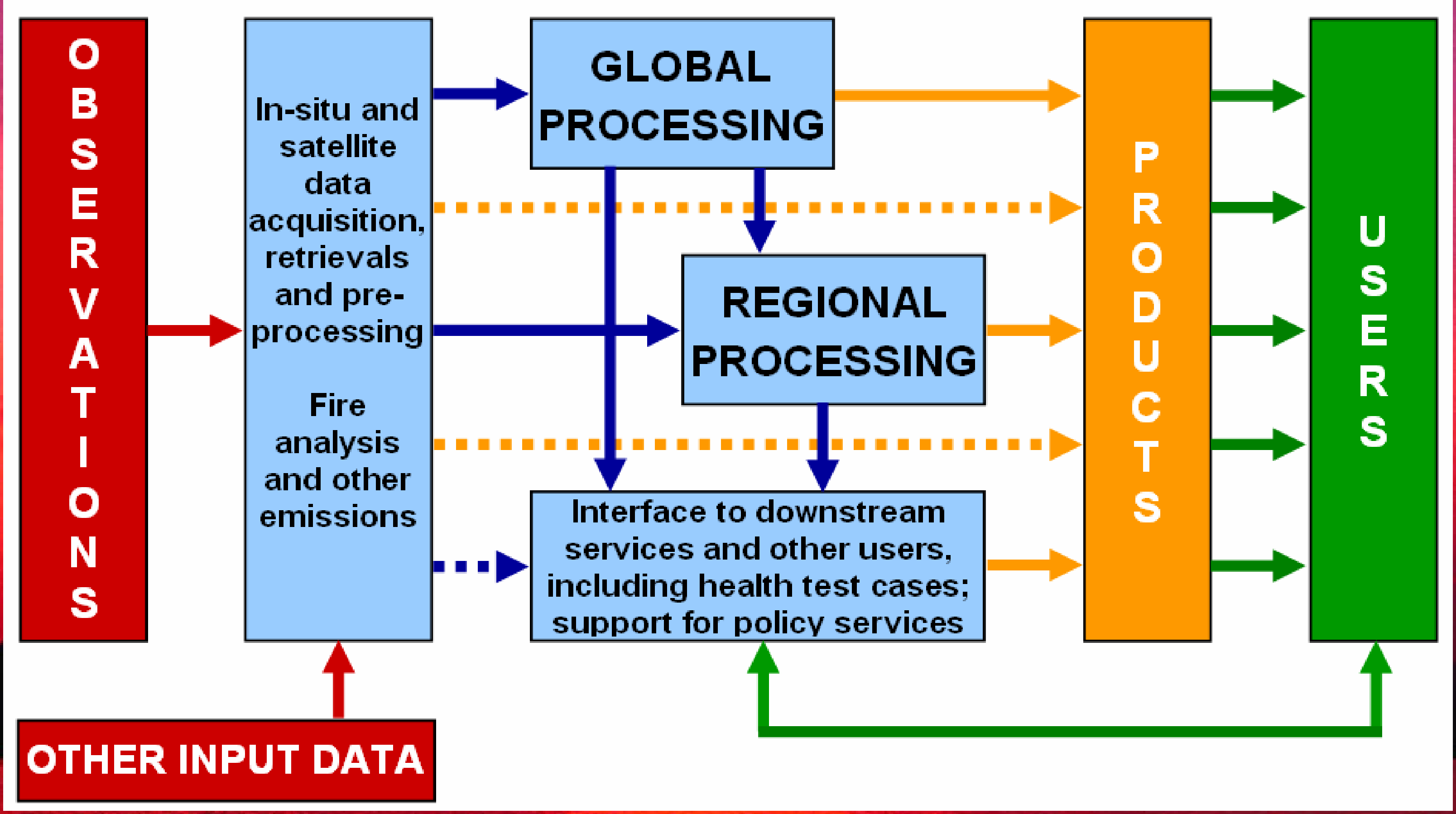
GEMS products at ECMWF

- Near-real-time global analyses and forecasts for reactive gases, aerosols and UV radiation
- Multi-year reanalyses of atmospheric composition (2003-2007) including greenhouse gases (CO2, methane), reactive gases (ozone, formaldehyde, CO, NOx) and aerosols (Sea salt, Desert dust, Black Carbon, Organic Matter, Sulphate)
- Web-hosting, archiving and verification of coordinated regional air-quality forecasts from ten systems

http://gems.ecmwf.int



MACC – Monitoring Atmospheric Composition and Climate



(Some) Validation metrics

- Quantitative:

 - Modified normalized mean bias

$$B'_n = \frac{2}{N}\sum_i \frac{f_i - o_i}{f_i + o_i}$$

 - Correlation coefficient

$$R = \frac{\frac{1}{N}\sum_i (f_i - \bar{f})(o_i - \bar{o})}{\sigma_f \sigma_o}$$

- Normalized Median Bias

$$NMedB = Median \sum_{i=1}^{region} \frac{(f_i - o_i)}{Median(o_i)}$$

For visualization:

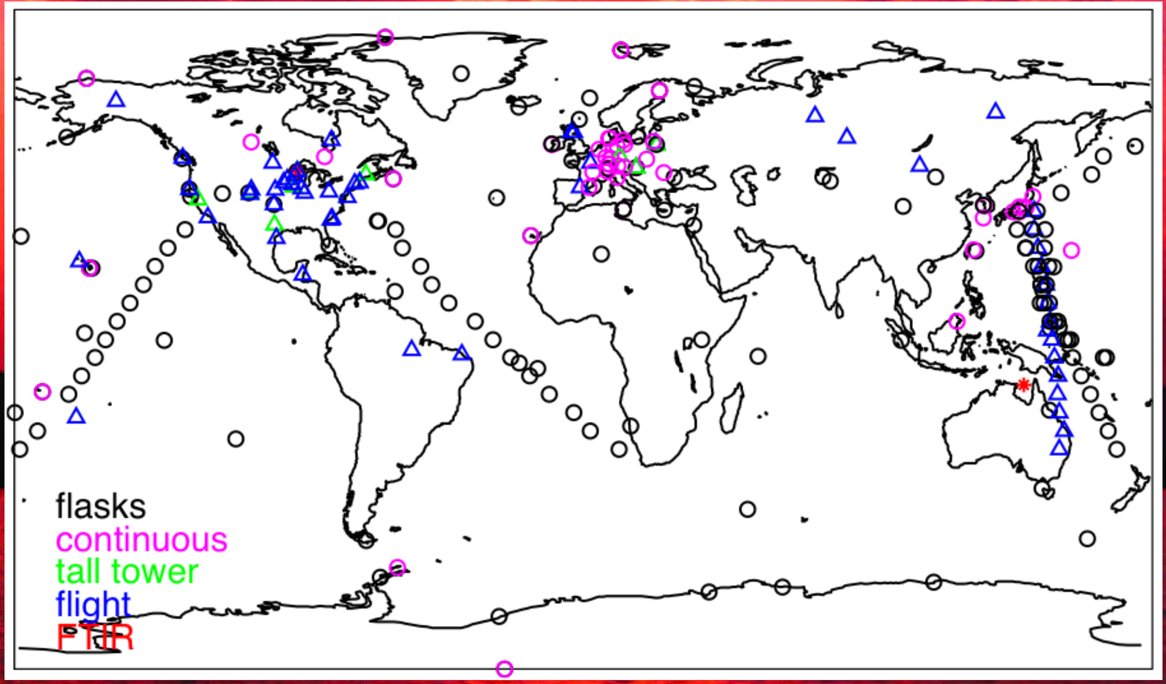
- Taylor diagrams (standard deviation and correlation)
- Scatterplots (bias and correlation)
- Line plots (time series or vertical profiles of bias and RMS)

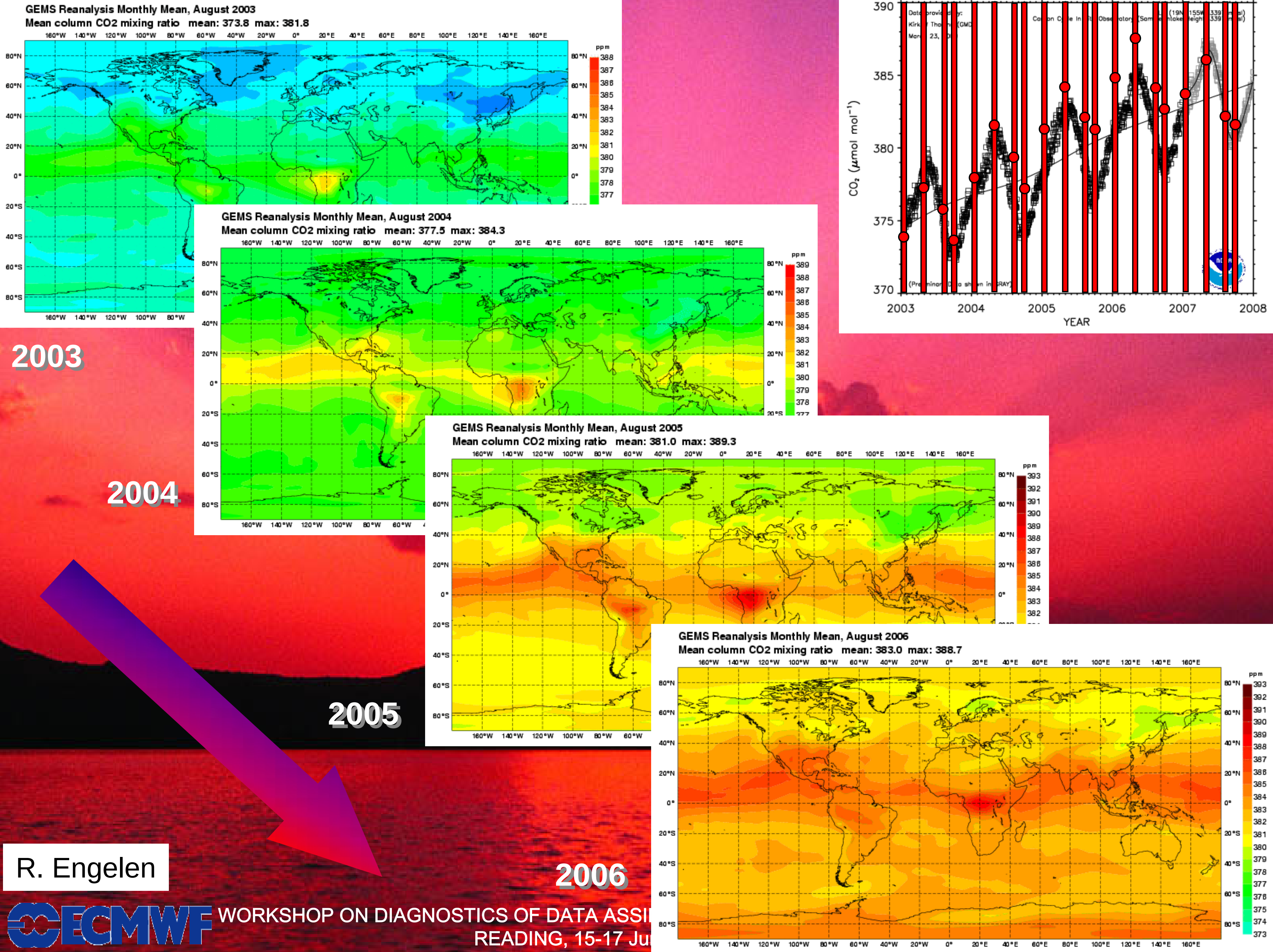
- Qualitative:

- Profile/cross section comparisons
- Maps

4D-var assimilation system for Greenhouse Gases

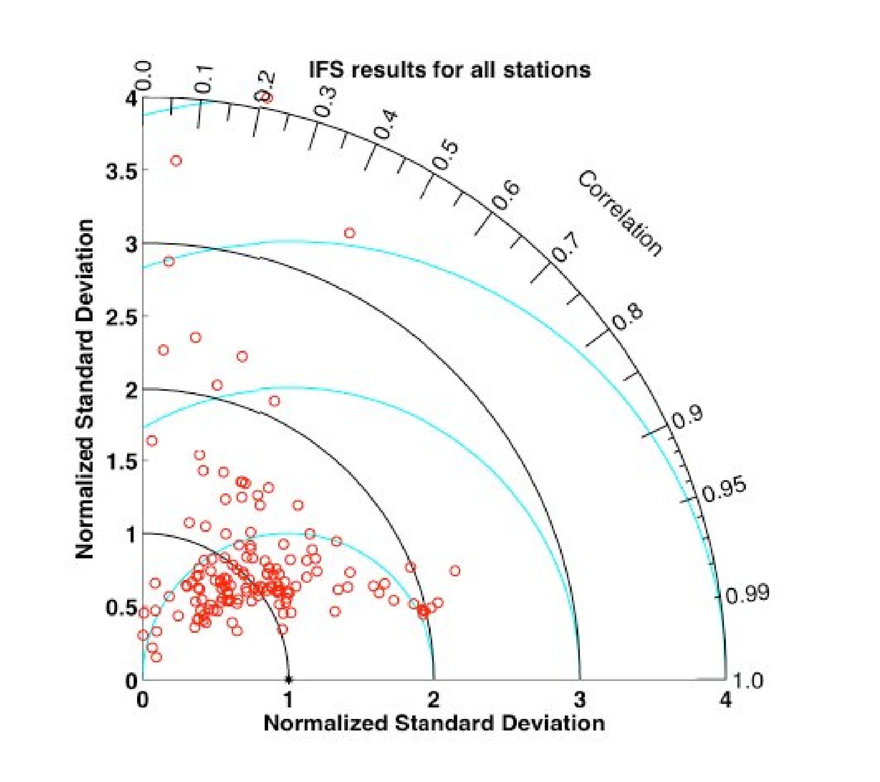
- Prognostic variables include CO2 and methane (also control variables)
- Background matrix calculated with NMC method
- 4D-Var analysis at T159 (~120 km) and 60 levels (same for GRG and AER)
- Assimilated observations: AIRS radiances for CO2 and SCHIAMACHY retrievals for CH4
- Verification observations: IASI CH4 retrievals, ground-based flux measurements, aircraft




GEMS Reanalysis Monthly Mean, August 2003
Mean column CO2 mixing ratio mean: 373.8 max: 381.8
GEMS Reanalysis Monthly Mean, August 2004
Mean column CO2 mixing ratio mean: 377.5 max: 384.3
GEMS Reanalysis Monthly Mean, August 2005
Mean column CO2 mixing ratio mean: 381.0 max: 389.3
GEMS Reanalysis Monthly Mean, August 2006
Mean column CO2 mixing ratio mean: 383.0 max: 388.7
ppm
2003
2004
2005
2006
CO_2 (μmol mol^{-1})
YEAR
R. Engelen
ECMWF
WORKSHOP ON DIAGNOSTICS OF DATA ASSI
READING, 15-17 Ju

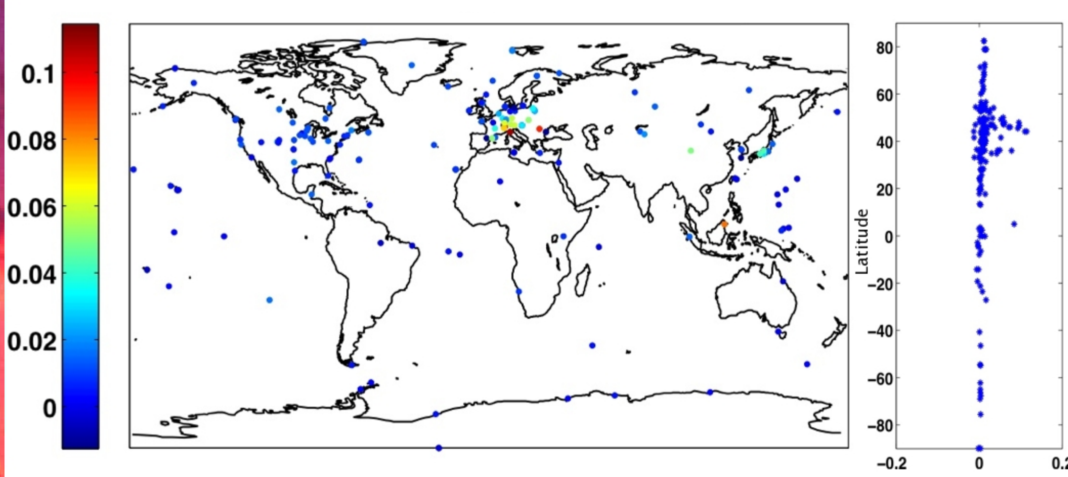
Comparison of IFS CO_2 fields with global in-situ data

- 4D IFS CO2 fields were sub-sampled to match available surface, tower, ship-based, and flight data
- The resultant timeseries were compared to observations
- Statistical results were summarized on Taylor diagrams (below), and with mapping (next slide)



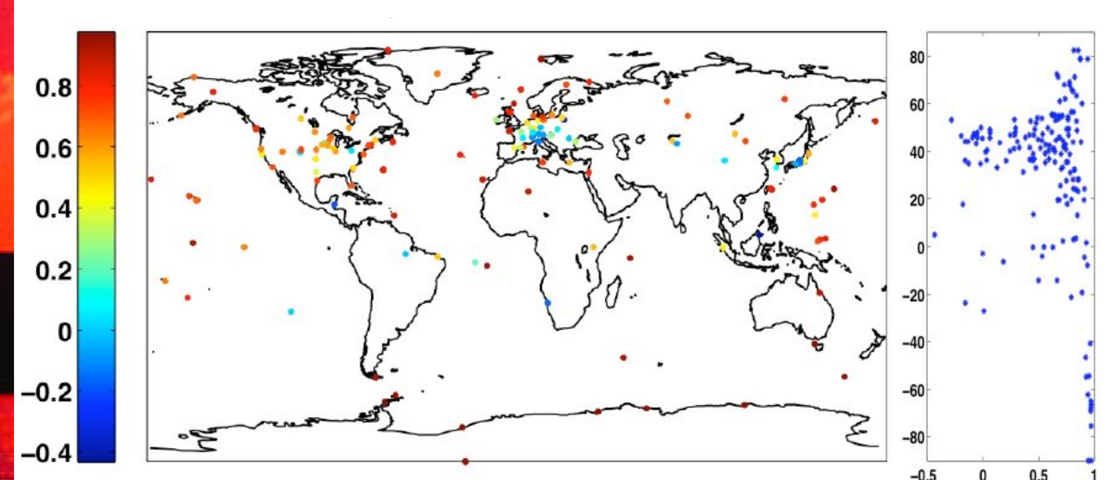
J. Marshall

Modified Normalized Mean Bias



- Up to 10% positive bias over Europe
- Southern hemisphere well-constrained, slightly positive tendency in northern hemisphere

Correlation coefficient



- Remote stations show good agreement
- Poor correlation over highly variable regions (Europe)

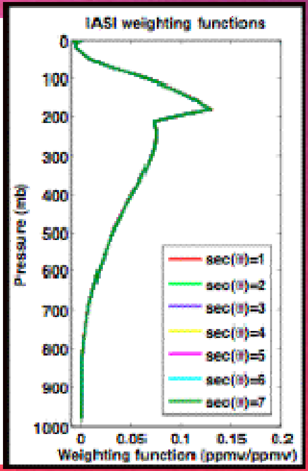
J. Marshall

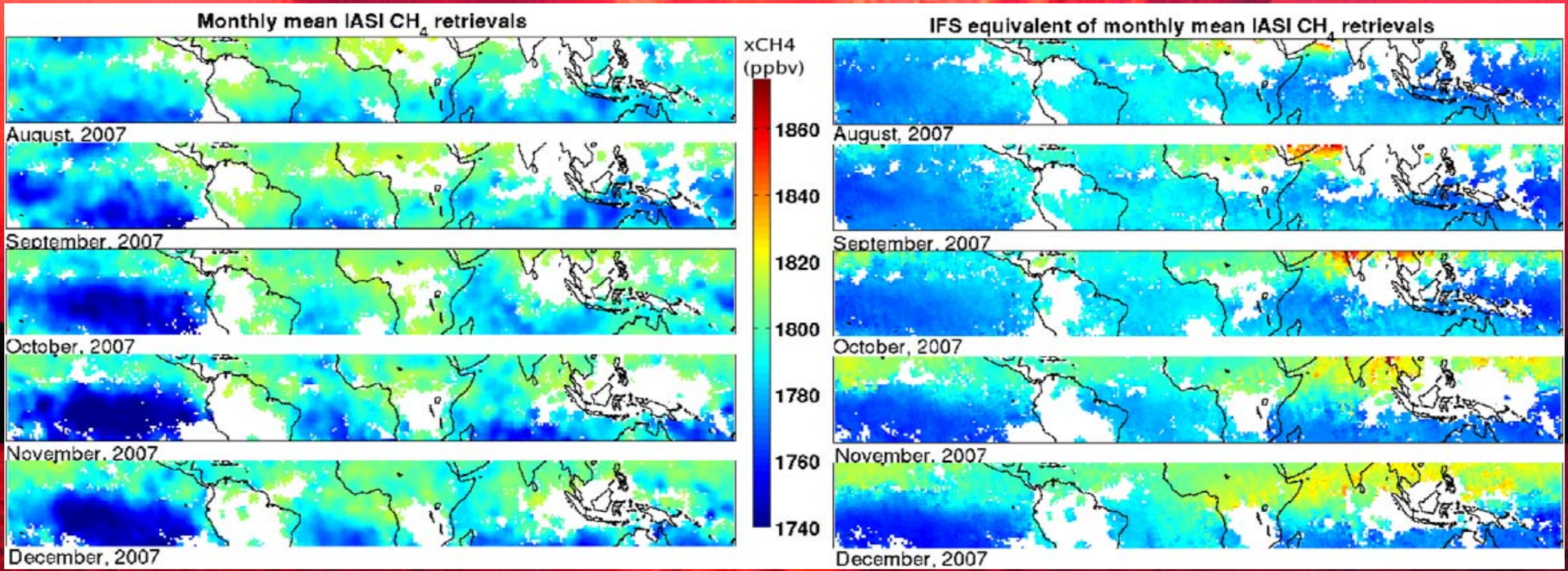
Conclusions from global comparisons

- Analyzed CO2 fields compare well with remote observations
- Positive bias and higher error seen over highly populated regions with heterogeneous fluxes
- Slight northern-hemisphere high bias, seems related to too weak seasonal cycle
- Trend shows some divergence over time
- Performance when considering non-surface data is comparable to that of an inversion system using only surface-based data

Comparison of IFS CH_4 fields with independent satellite retrievals (from IASI)

- 4D IFS fields were sub-sampled in time and space to match individual retrievals from an independent satellite
- The appropriate weighting function was applied (shown)
- Monthly mean maps were compared for spatial and temporal correlation





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4D-var assimilation system for aerosols

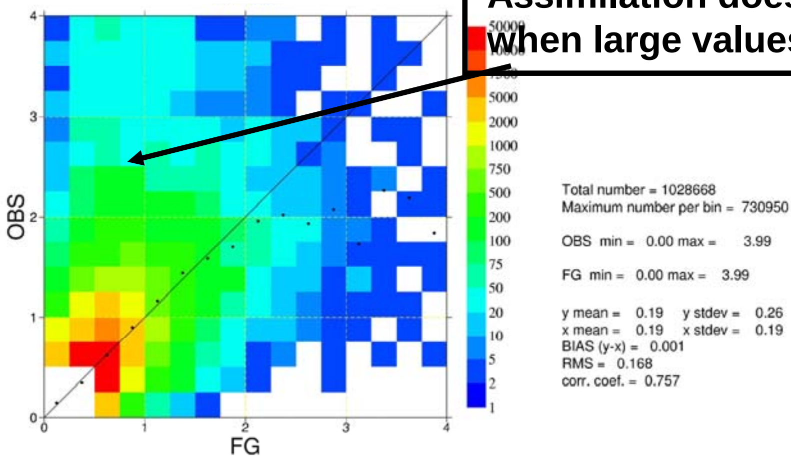
- Aerosol prognostic variables include 3 bins for desert dust, 3 bins for sea-salt, hydrophobic and hydrophilic organic matter, hydrophobic and hydrophilic black carbon, and sulphate.
- The control variable is formulated in terms of the total aerosol mixing ratio
- Background error statistics have been computed using the NMC method
- Assimilated observations: MODIS Aerosol Optical Depths (AODs) at 550 nm over land and ocean. Observation errors over ocean are prescribed as functions of the satellite scattering angle. Errors over land are assigned as 50% of the optical depth value.
- Validation datasets: optical depths from the AErosol Robotic NETwork (AERONET), AEROCE (U. of Miami), compilation datasets.
- Verified variables: AOD, Angström exponent (α defined from $\left({}^{AOD_1}\!/_{AOD_2}\right)=\left({}^{\lambda_1}\!/_{\lambda_2}\right)^{-\alpha}$)

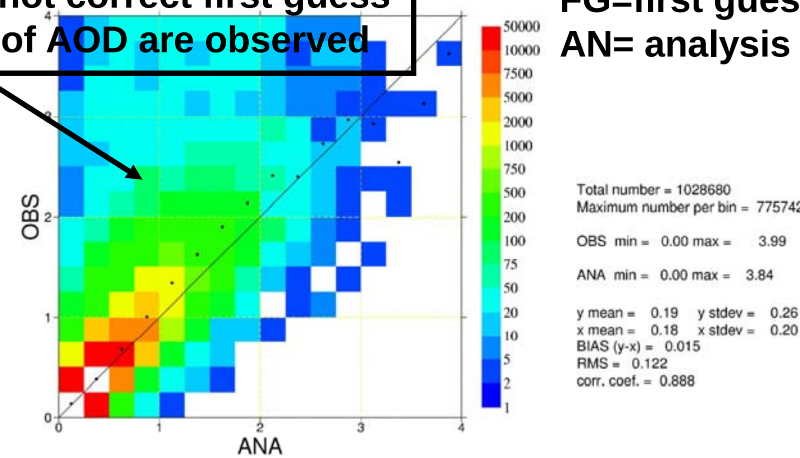
Departure statistics for the aerosol analysis

Not an independent verification but a very helpful tool for a quick check of the system performance!

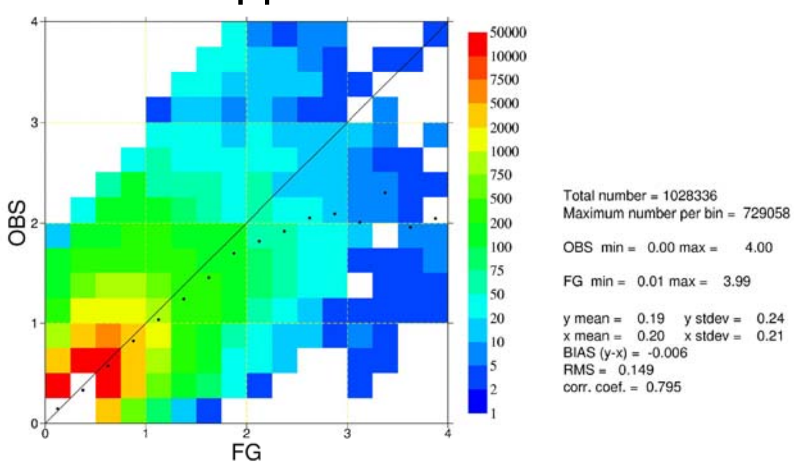
Assimilation does not correct first guess when large values of AOD are observed

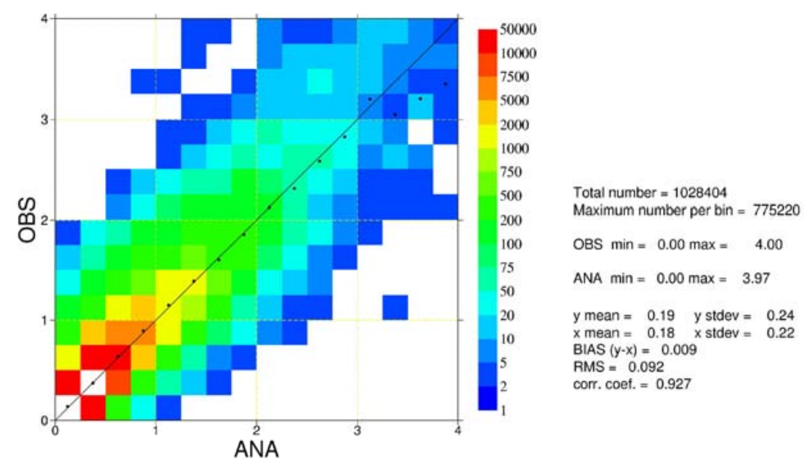
FG=first guess
AN= analysis



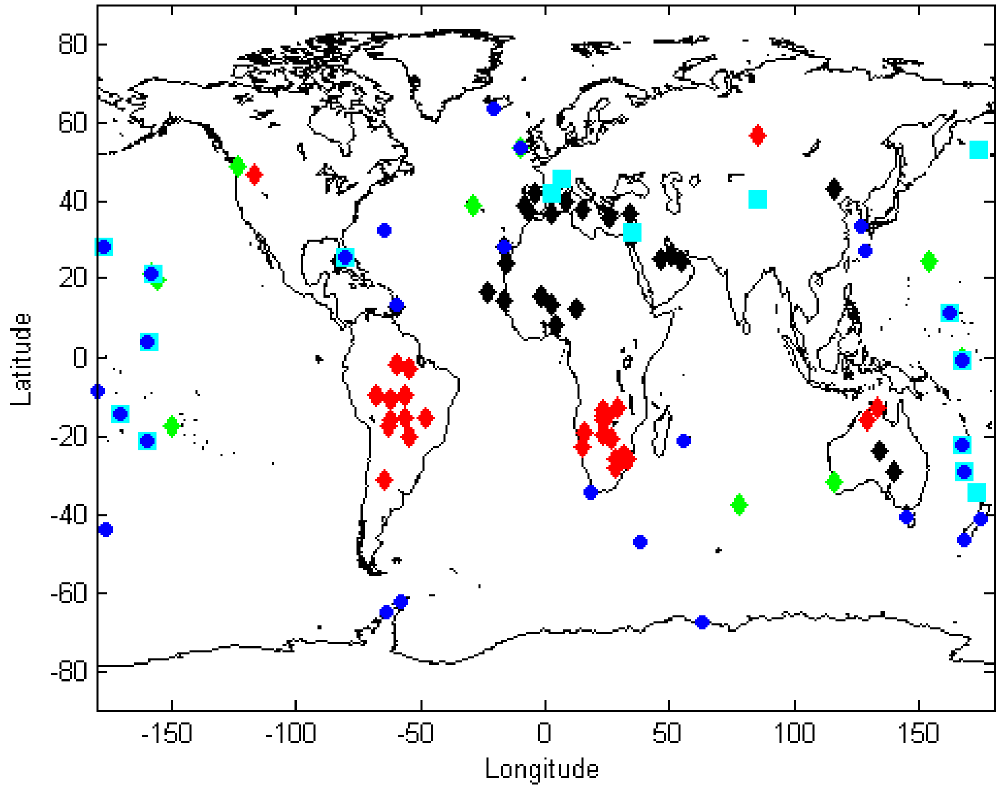


This behaviour is improved when observation errors for optical depths larger than 1 are capped to 0.4





Independent aerosol observations



Optical Depth 550 nm & Angström Exponent (AERONET)

Surface Concentration DD (AEROCE, U. de Miami)

Total Deposition (Ginoux et al, 2001)

Desert Dust Stations

Biomass Burning Stations

Sea Salt Stations

AERONET Stations where a species dominates the total optical depth for at least 4 month.

Global statistics using AERONET

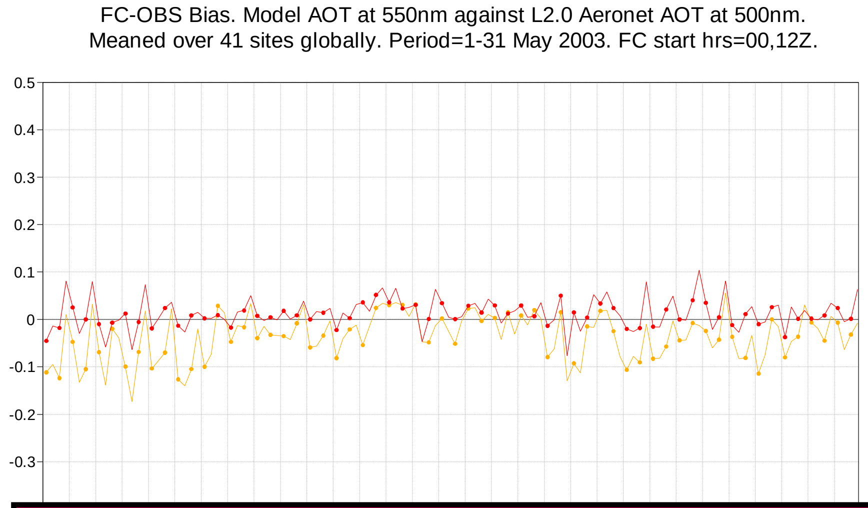
	FCST 2003	FCST 2004	ASSIM 2003	ASSIM 2004	AeroCom Median 2000	MODIS terra 2003	MODIS terra 2004	MODIS aqua 2003	MODIS aqua 2004
Aeronet AOD	*0.22*	*0.22*	*0.22*	*0.22*	*0.18*	*0.22*	*0.22*	*0.22*	*0.22*
# N months	*1225*	*1422*	*1225*	*1422*	*731*	*1173*	*748*	*1143*	*1292*
Model AOD	0.24	0.26	0.27	0.27	0.16	0.22	0.22	0.20	0.20
Correlation	0.68	0.69	0.82	0.82	0.77	0.80	0.80	0.79	0.78
RMS	0.13	0.14	0.11	0.12	0.09	0.11	0.12	0.11	0.12
Std Mod/Obs	0.76	0.73	0.81	0.79	0.80	0.91	0.86	0.89	0.93
Seasonal r	0.75	0.76	0.80	0.80	0.73	0.80	0.72	0.81	0.79
Spatial r	0.71	0.73	0.78	0.81	0.65	0.77	0.74	0.80	0.81

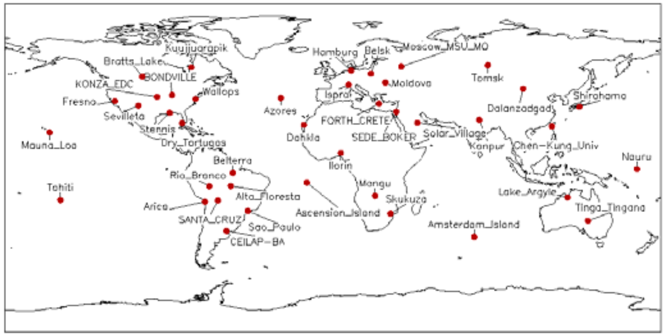
= mean value = correlation = Root Mean Square

- Global statistics show that the analysis (ASSIM) has a positive bias with respect to the AERONET data which is larger than that of the forecast without assimilation (FCST) while having much higher correlation and lower RMS with respect to the same dataset.
- Good performance of the analysis in terms of seasonal and spatial correlation.

M. Schulz

More (global) comparisons with AERONET on a subset of stations (May 2003)

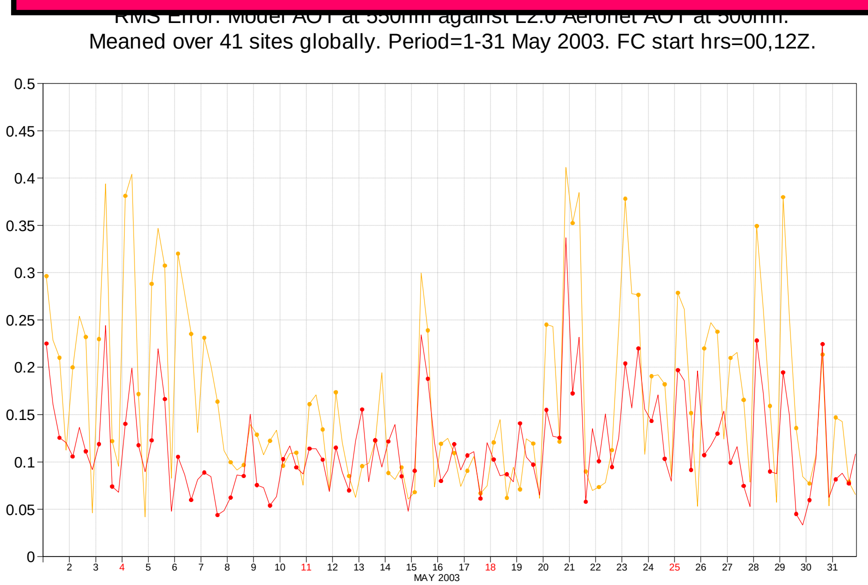




Analysis (red) shows lower bias and lower RMS wrt AERONET optical

Conclusions from verification may depend on choice of data set!!

(dark yellow)



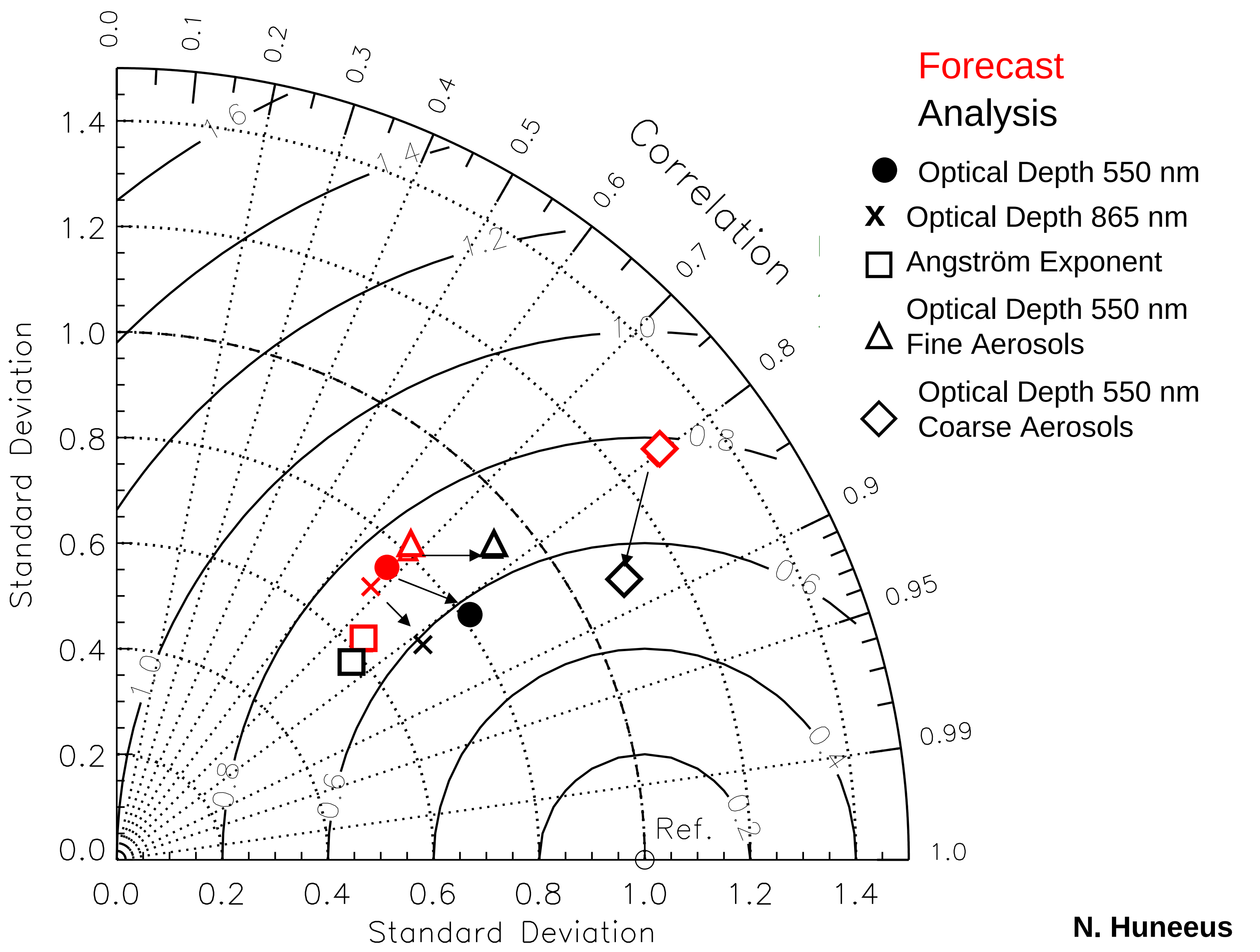
Average bias (over 41 stations):
0.012 (ASSIM) vs -0.036 (FCST)

RMS:
0.117 (ASSIM) vs 0.164 (FCST)

Analysis

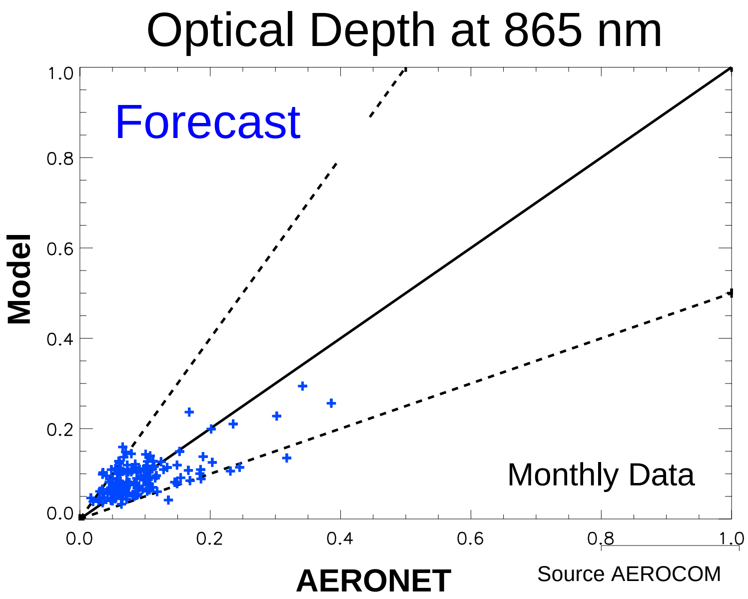
Free-running forecast

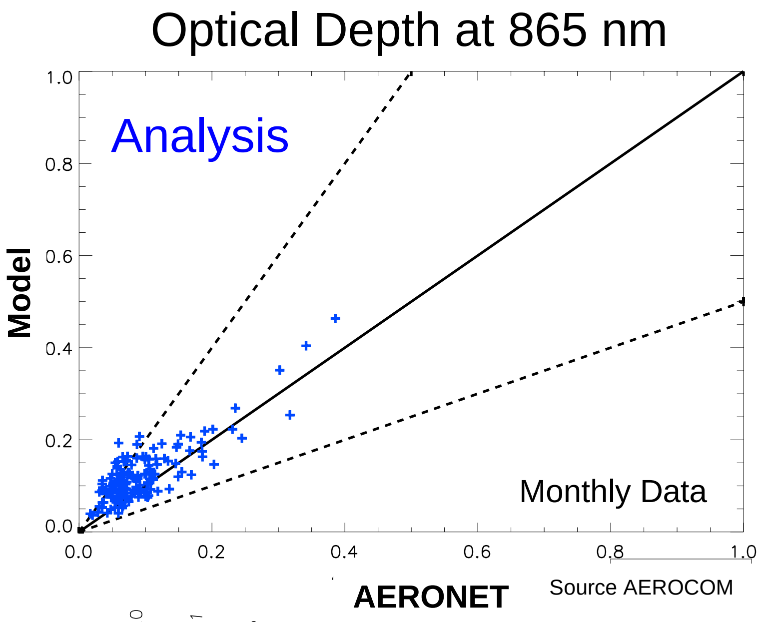
Taylor diagram for all AERONET Sites (2003)

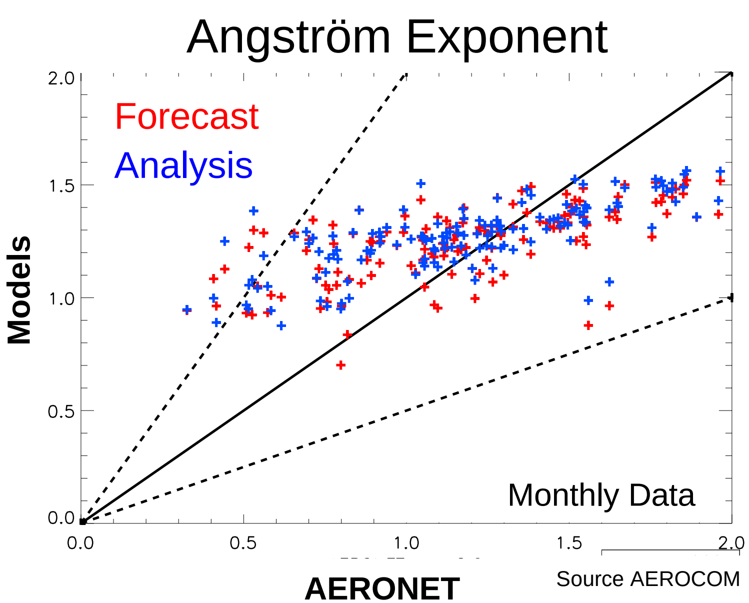


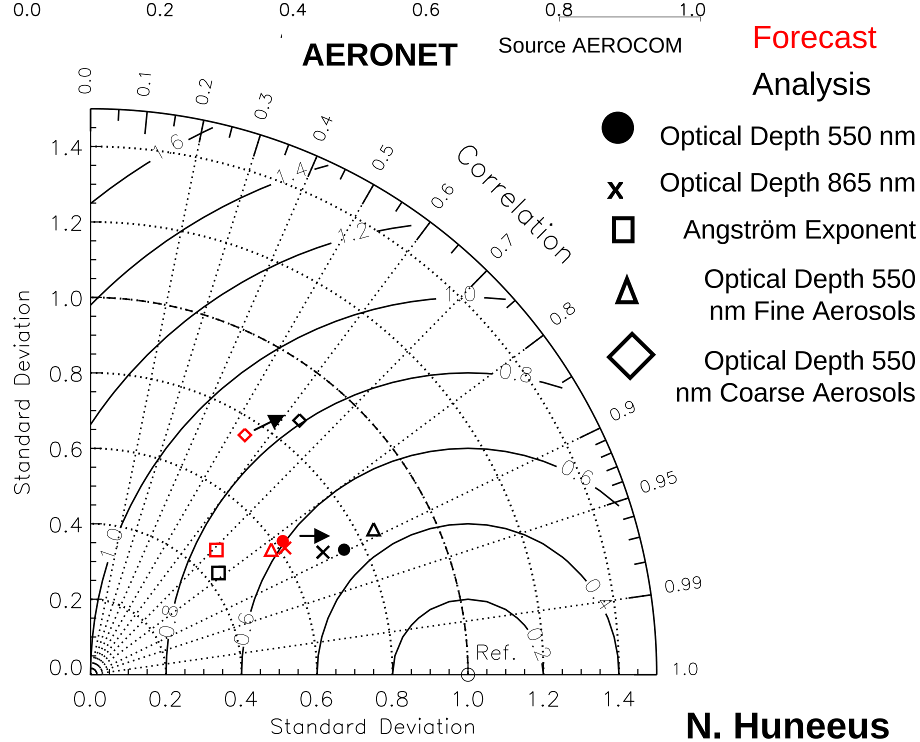
N. Huneeus

Biomass Burning Sites



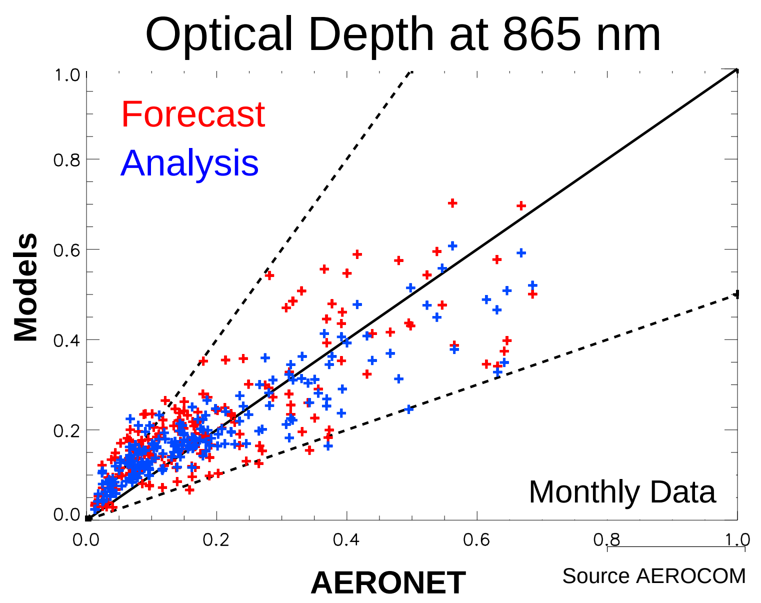


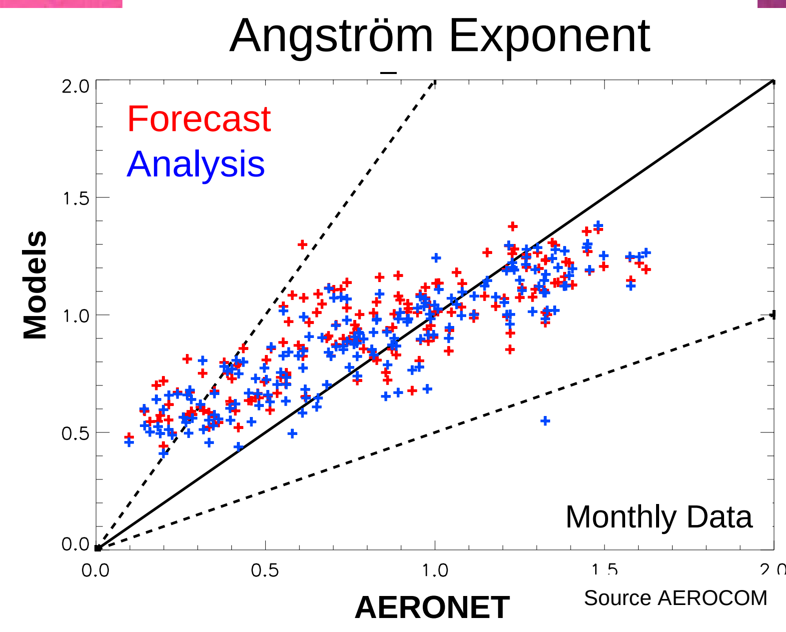


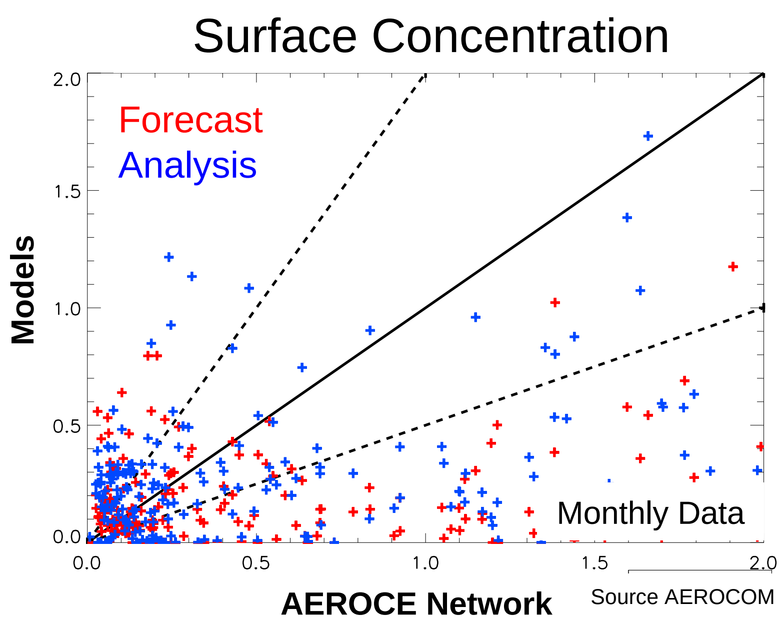


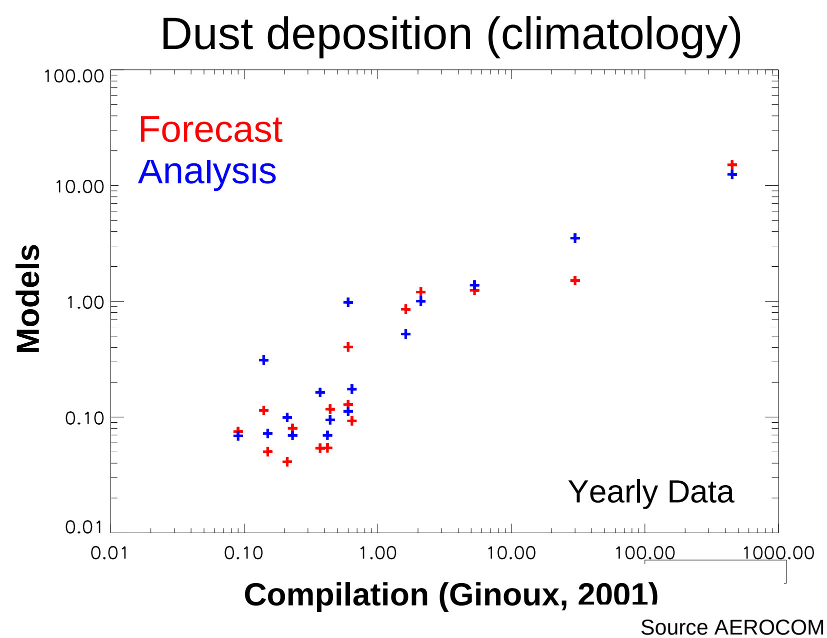
N. Huneeus

Desert Dust Sites









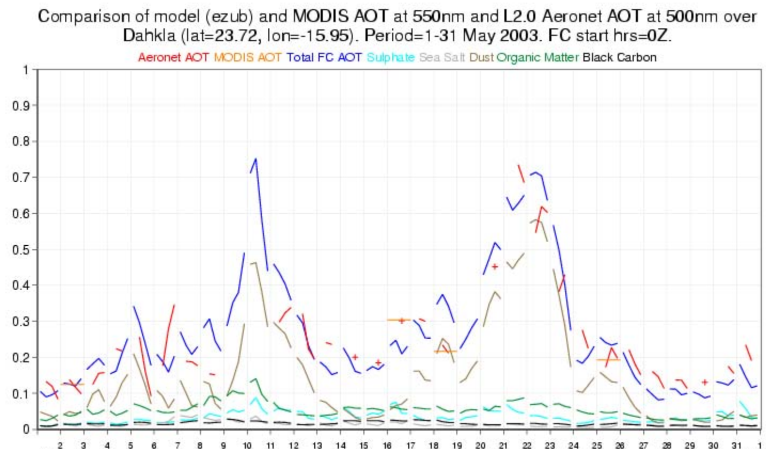
N. Huneeus

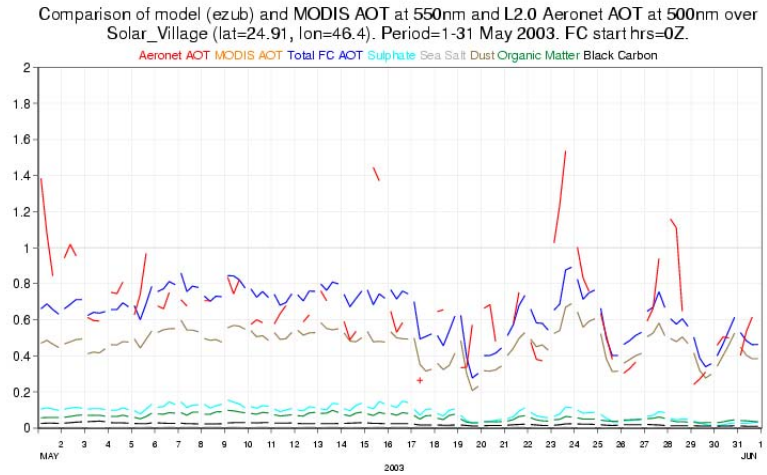
Conclusions from global comparisons

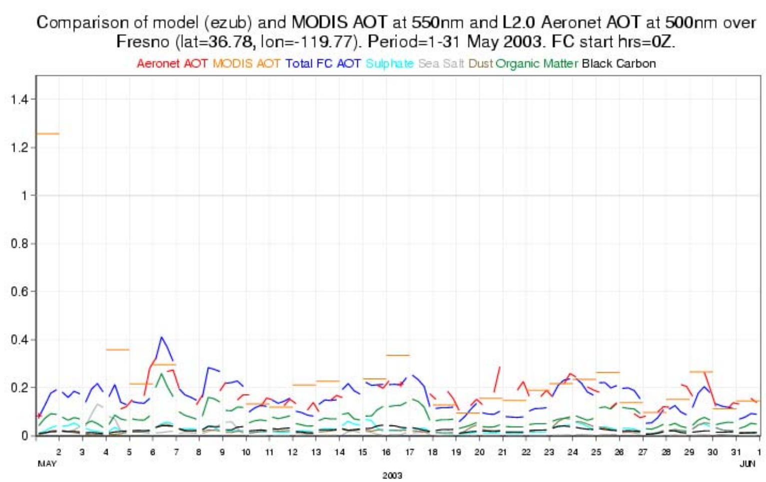
- Significant improvement in column integrated aerosol variables in terms of correlation and RMS. A positive bias is present in the analysis.
- Assimilation of AOD at 550 nm improves also AOD at 865 nm.
- Improvement of AOD at 550 and 865 nm does not translates into improvement of Angström exponent suggesting that assimilation acts on correcting total aerosol burden rather than size distribution.
- Overestimation of the Angström exponent for coarse aerosols indicates smaller particles in the model.
- Too much fine mode sea salt represented in the model
- Not enough Desert Dust is emitted and too much fine Desert Dust is transported far off source regions.

Site comparisons (May 2003)

- Dust-dominated sites (Dakla and Solar Village) show good agreement between the analysis and AERONET despite the lack of MODIS data over these sites







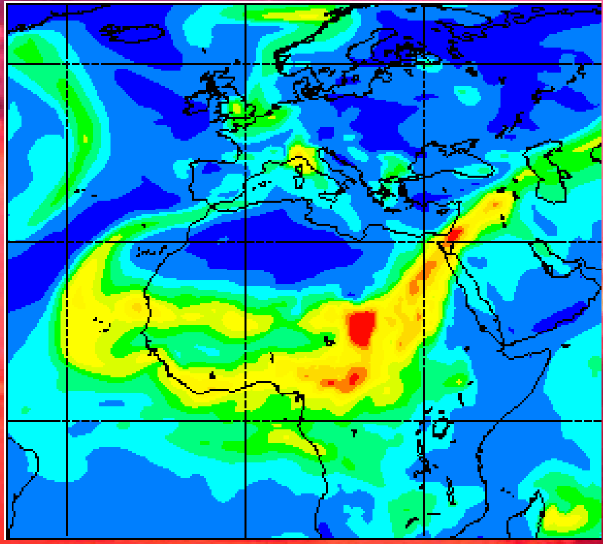
- AERONET data for Fresno (CA) also confirm a good performance of the analysis

AERONET
MODIS AOD
MODEL AOD

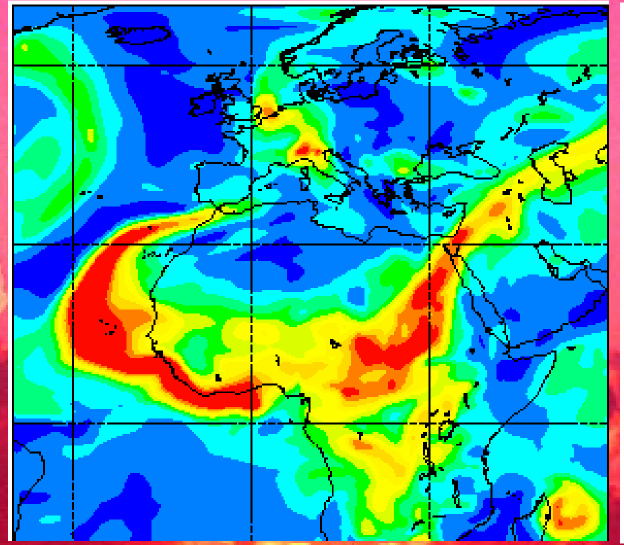
Sulphate
Sea-salt
Dust
Organic
Black carbon

Saharan dust outbreak: 6 March 2006

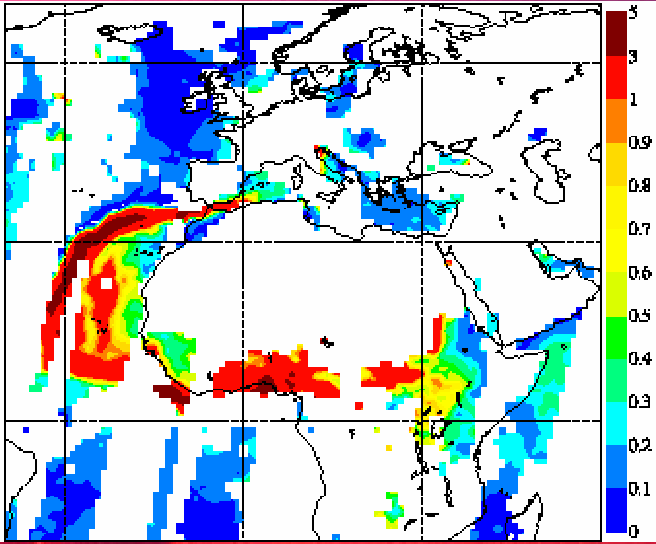
Model simulation



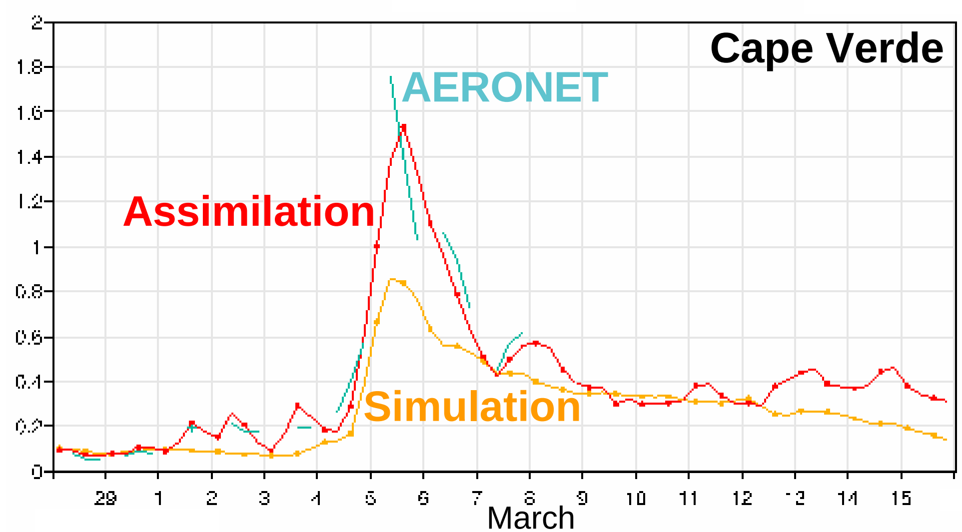
Assimilation

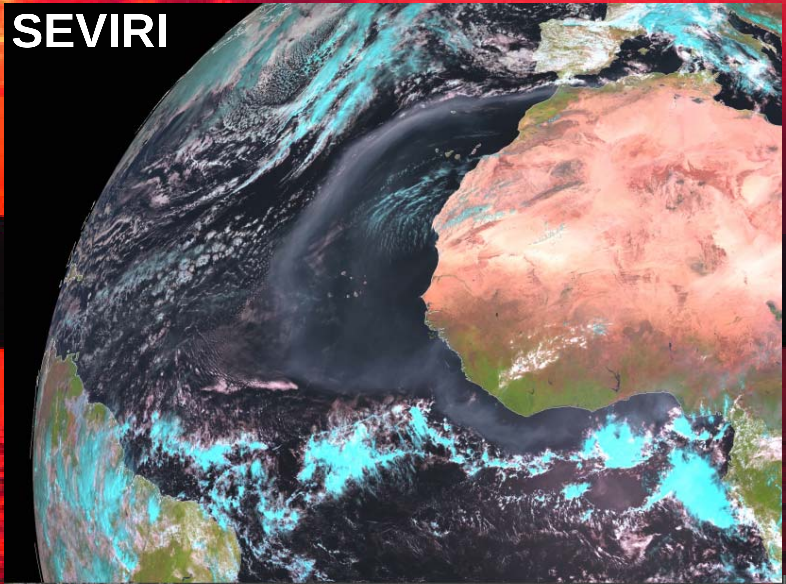


MODIS

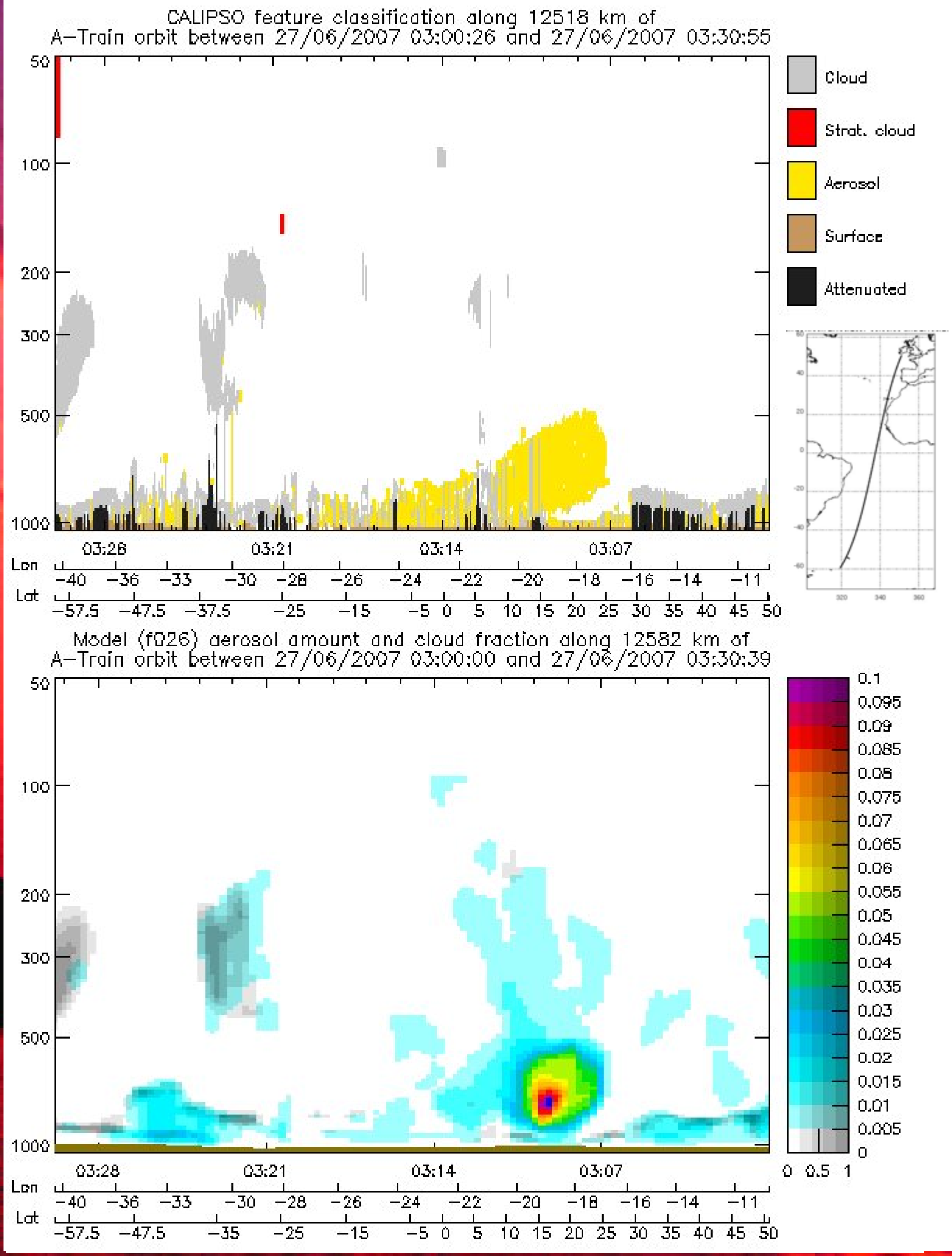


Aerosol optical depth at 550nm





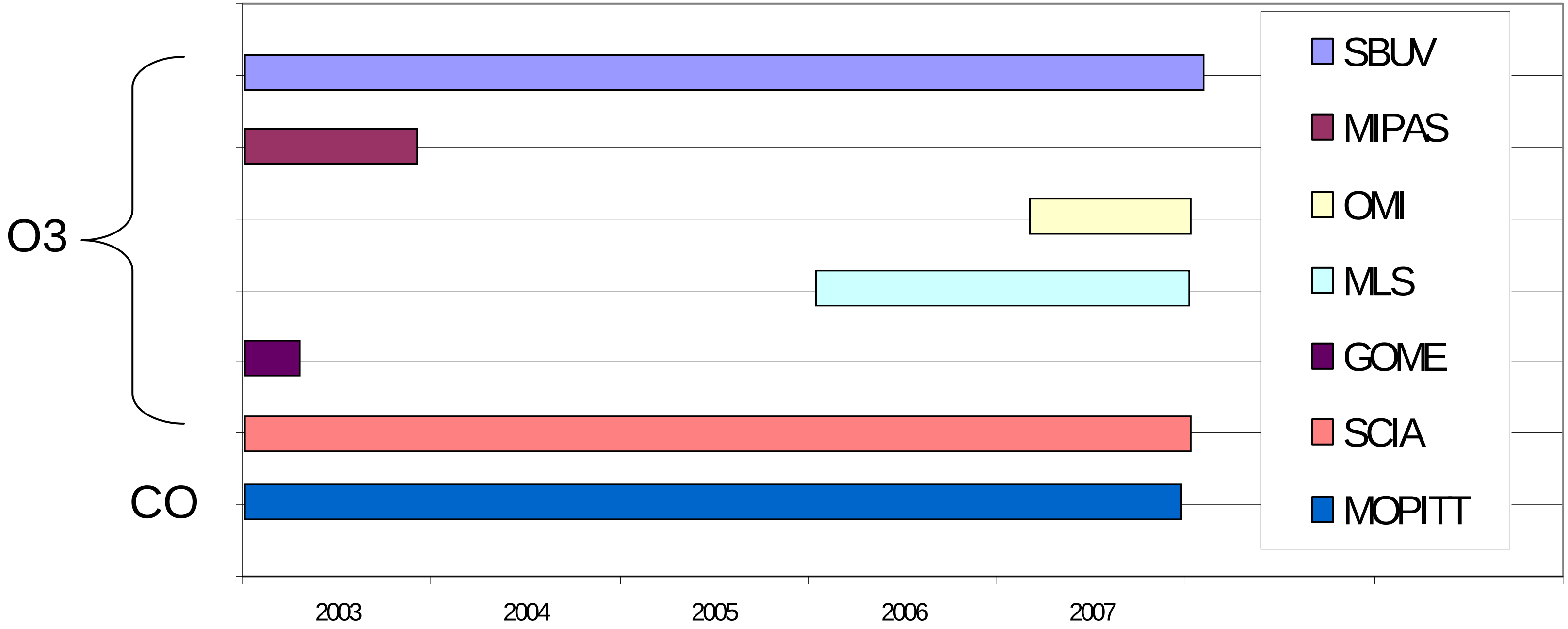
Comparison with CALIPSO aerosol mask



- General good agreement on the vertical but no improvement with respect to forecast without assimilation
- Too much aerosol is present in the upper troposphere in the model and analysis (likely to depend on interaction between convection/vertical diffusion and aerosol transport)
- Observations in the analysis do not constrain the vertical profile (only a total aerosol mass adjustment)
- Plans to compare extinction profiles

4D-var assimilation system for Reactive Gases

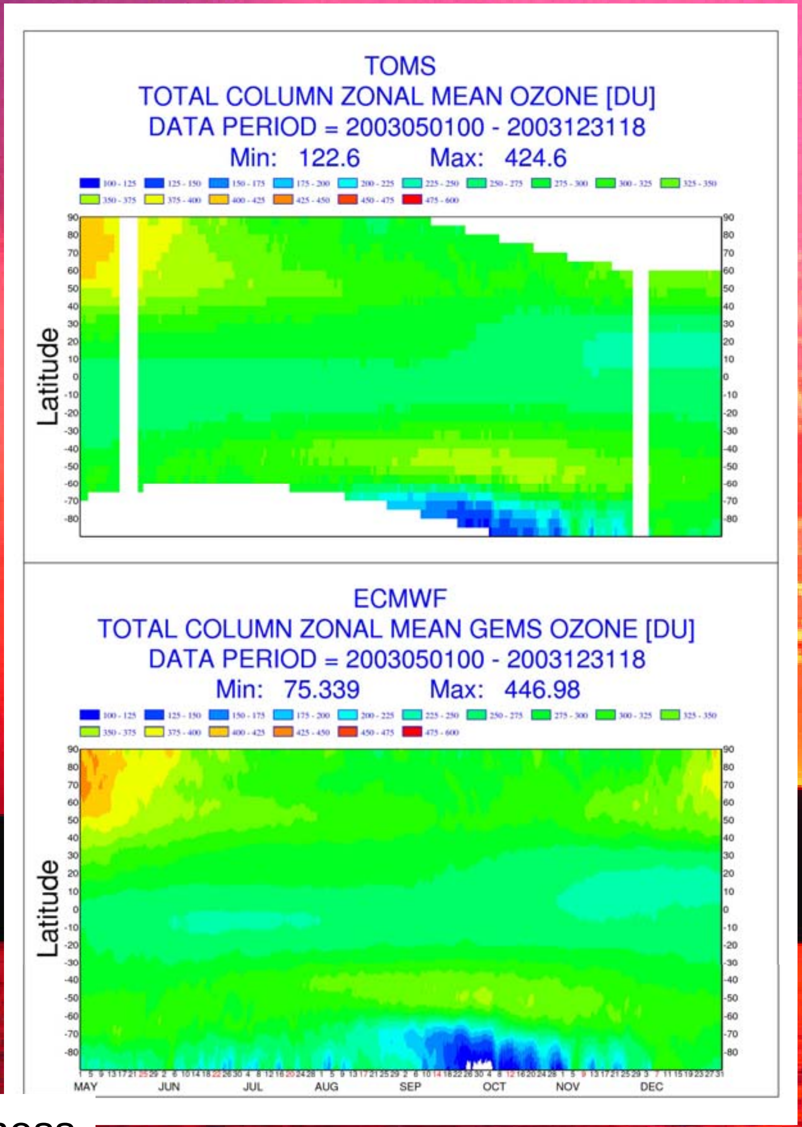
- GEMS –reanalysis (2003-2007): O3, CO, NOx, Formaldehyde
- Chemical model MOZART coupled to IFS (exchange of chemical tendencies and meteorological fields every hour)
- Observations used (O3 and CO):



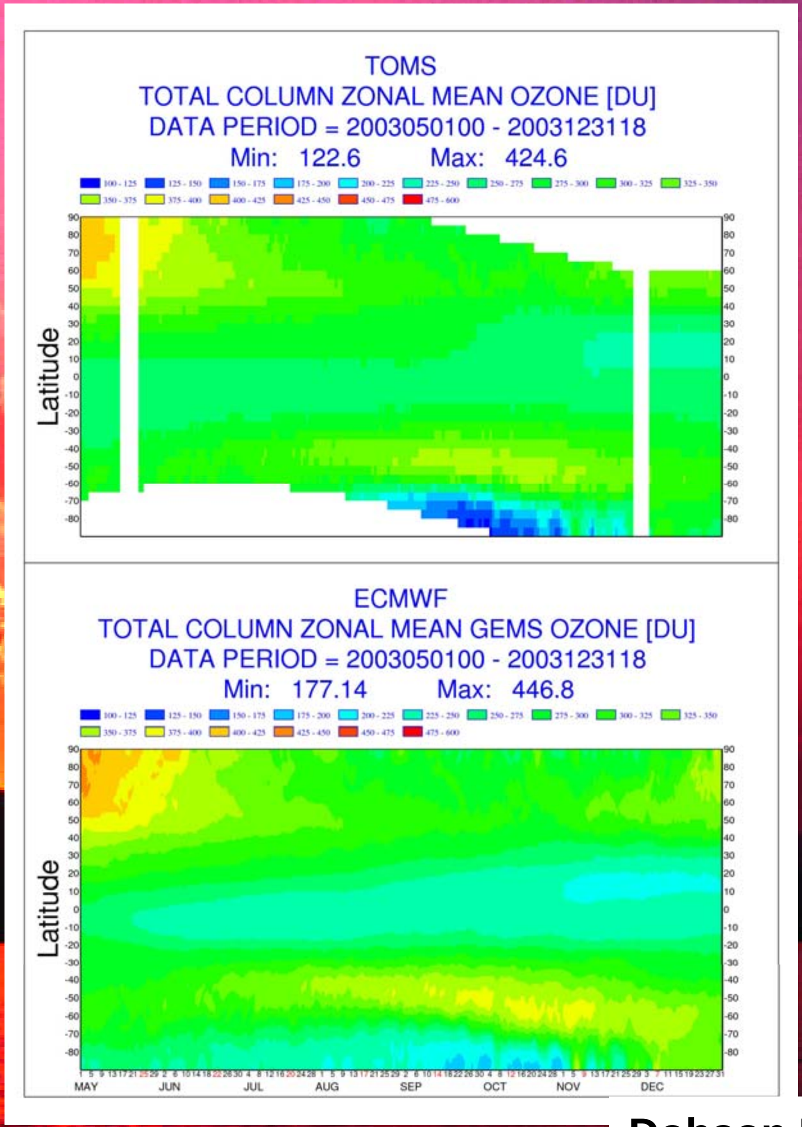
- Verifying observations: TOMS, SCHIAMACHY,GAW surface O3 and CO, MOZAIC flight data (vertical profiles)

Timeseries of zonal mean total column ozone

Assimilation run



Control run

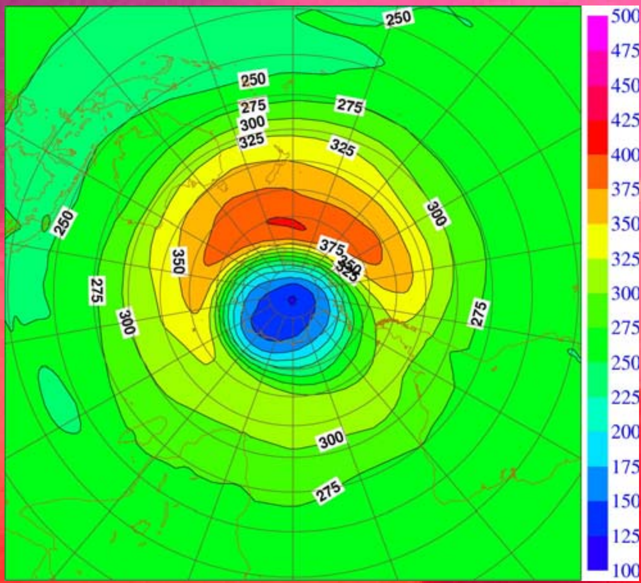


A. Inness

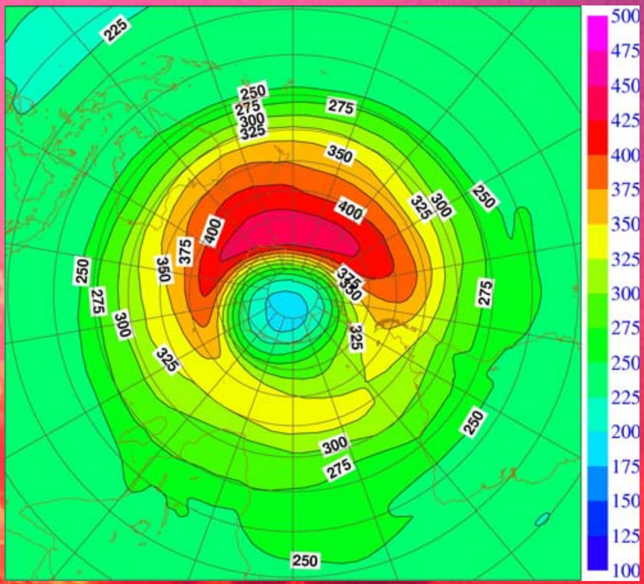
Dobson Units

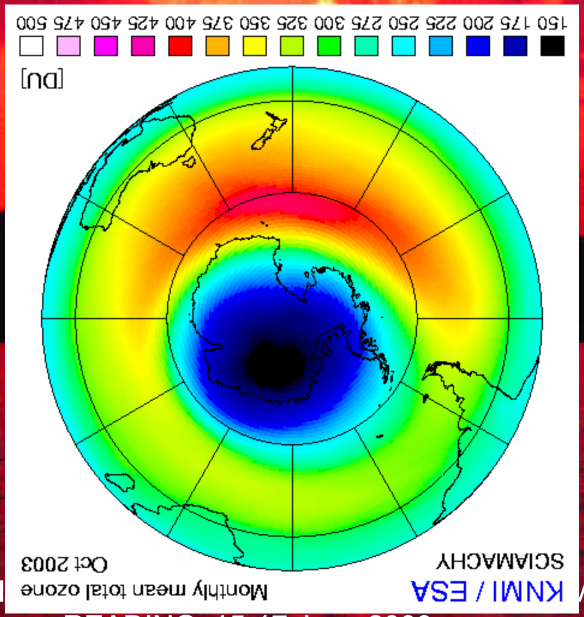
Mean total column ozone October 2003

Assimilation run



Control run





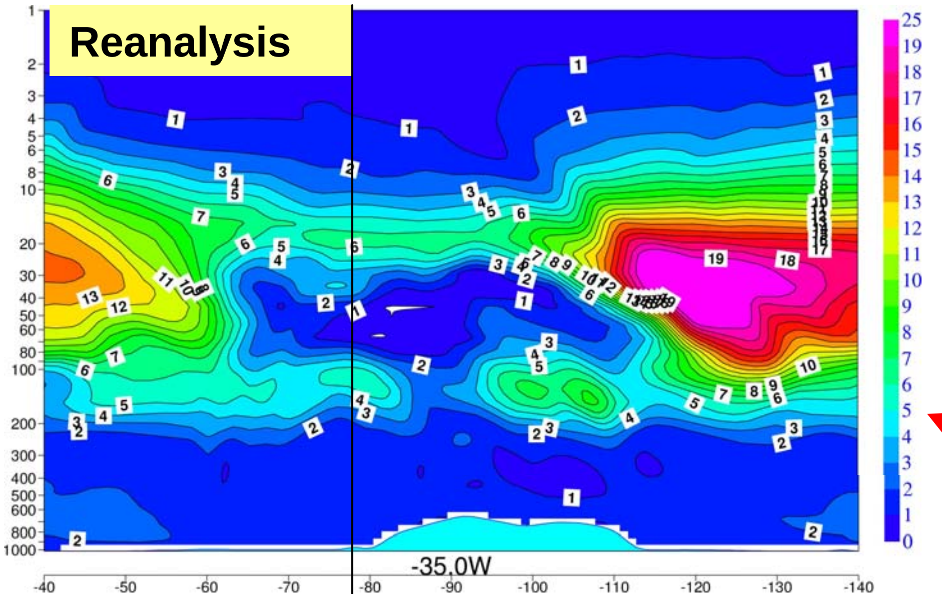
SCIAMACHY

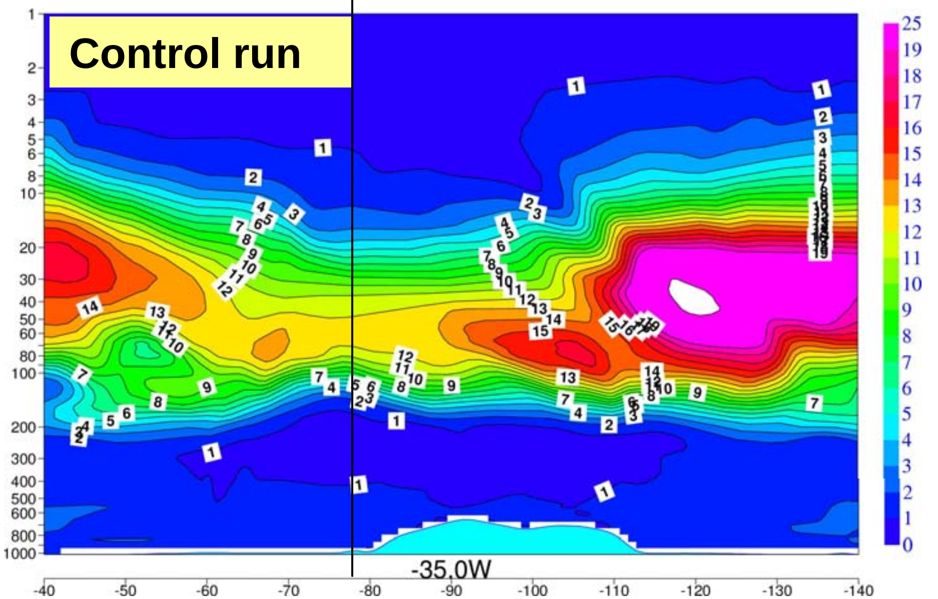
(Different colour scale)

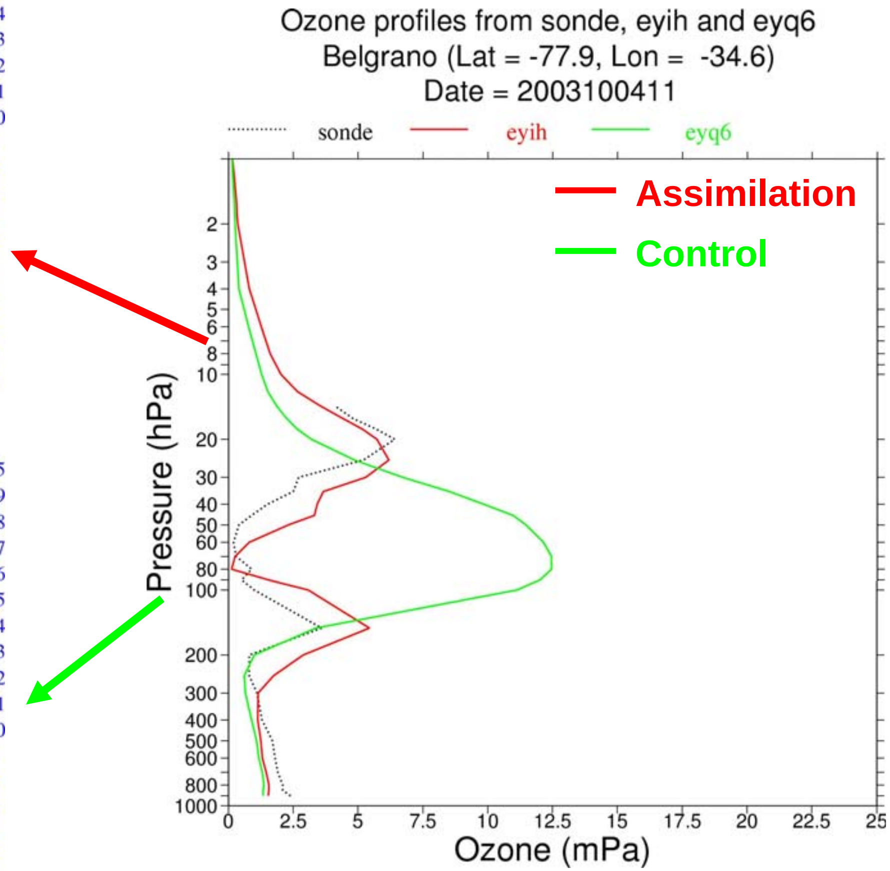
A. Inness

Dobson Units

Cross section along 35E over South Pole, 4 Oct 2003

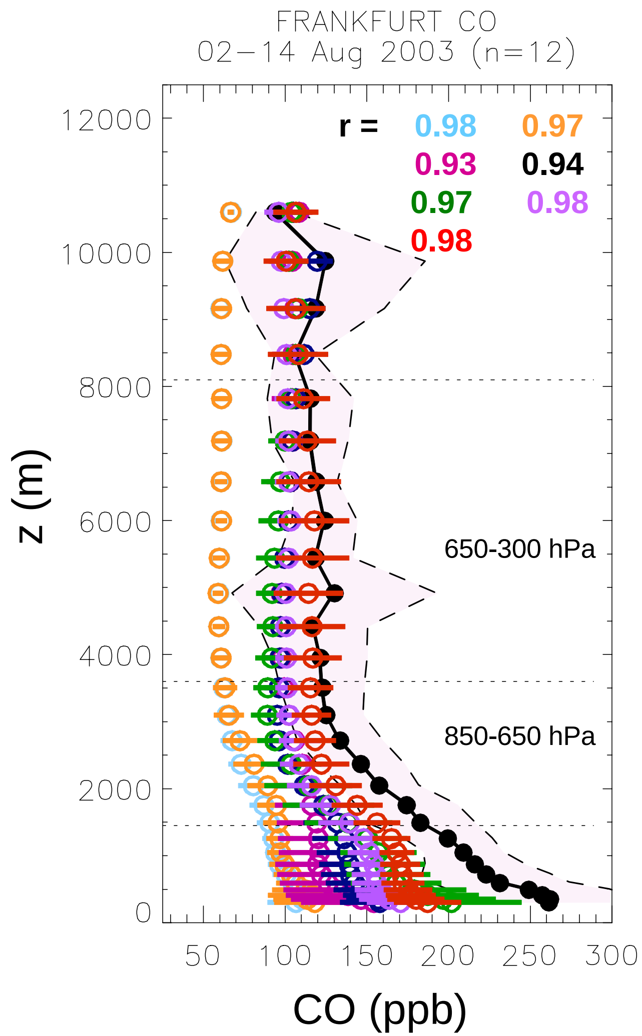






A. Inness

Vertical CO profiles above Frankfurt during the summer 2003 heat wave



MOZART+IFS+assim (eyih)

MOZART+IFS (eyq6) - coupled

MOZART high res: 1.125º X 1.125º

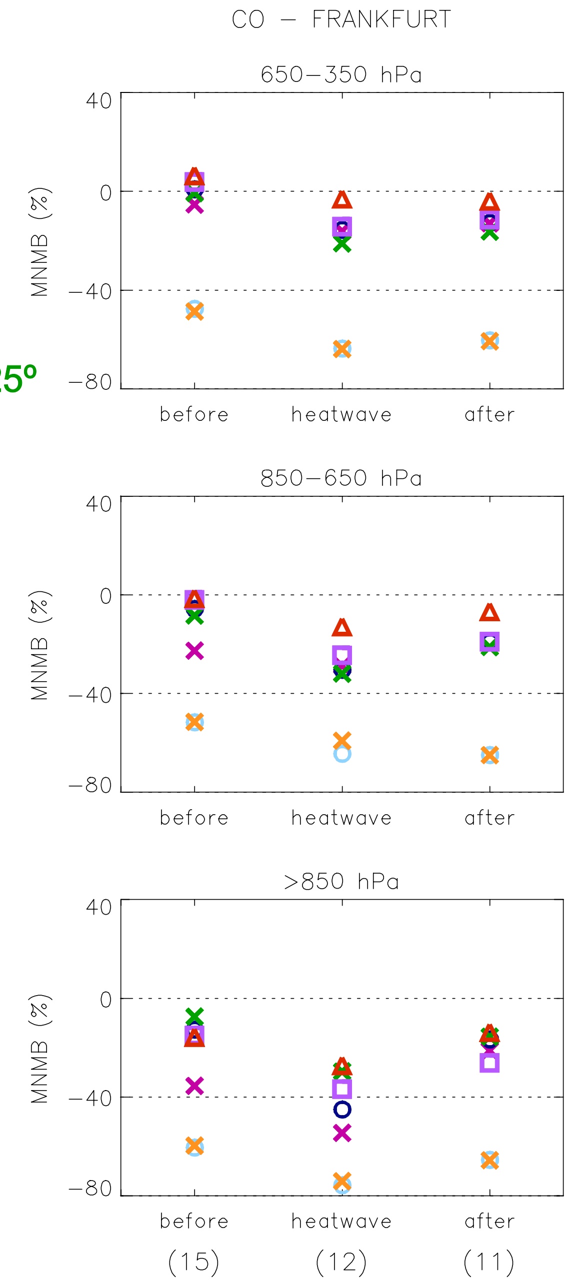
MOZART: 1.875º X 1.895º

MOCAGE: 2º lon X 2º lat

TM5 zoom1º X 1º over the European domain

TM5 3º lon X 2º lat

MOZAIC–aircraft observations

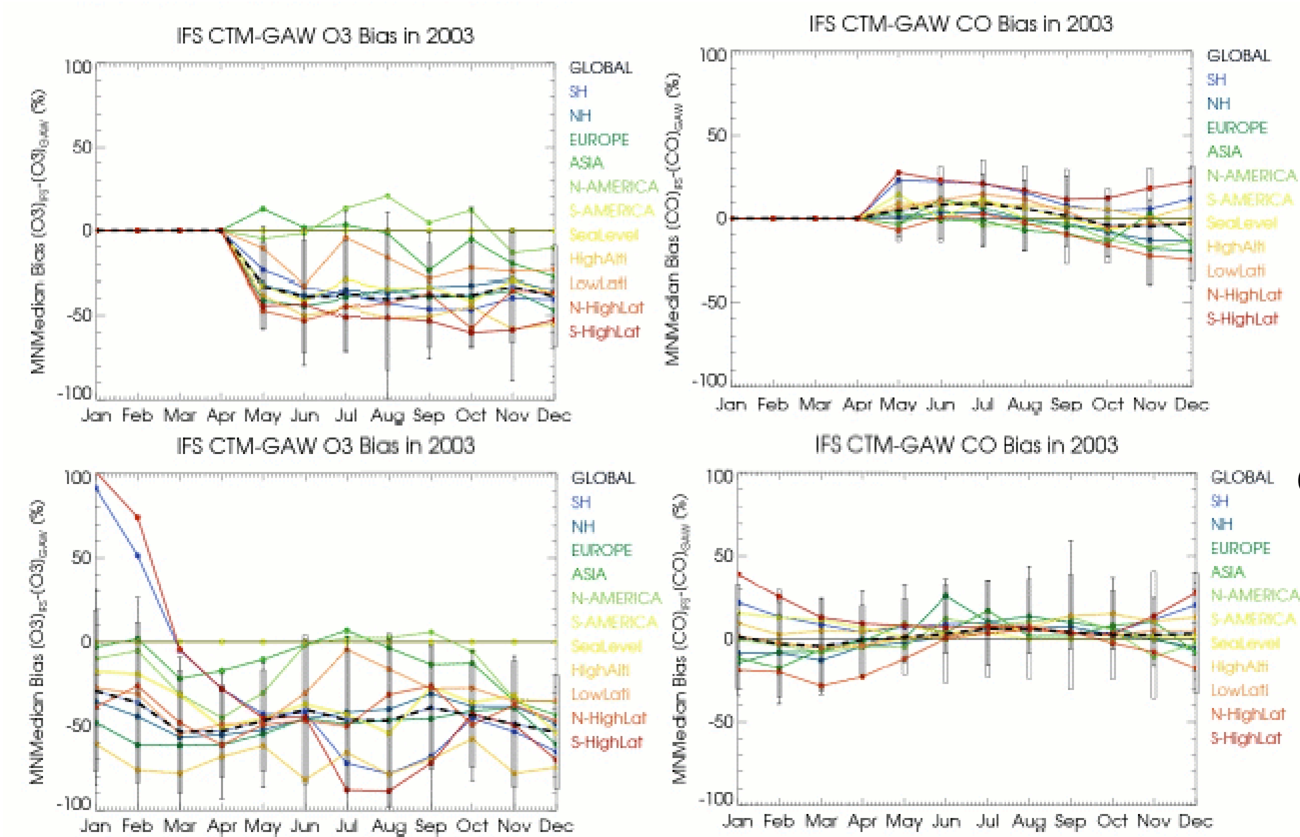


- **GEMS-GRG coupled system** (MOZART+IFS):
  - exchange of meteo fields and chem tendencies at 1h intervals
  - Assimilation of column retrievals of CO from MOPITT

C. Ordóñez

Comparison of GRG runs with O3 and CO surface measurements

Normalized median bias



Control run, no assim

GEMS reanalysis

$$NMedB = Median\sum_{i=1}^{region}\frac{(f_i - o_i)}{Median(o_i)}$$

E. Katragkou/H. Flentje

Choosing the right model level for comparison with CO (O3) observations from GAW mountain stations

- GAW stations are supposed to be horizontally representative for a grid box size of 120 km but what is their vertical representativeness, i.e. which model level to compare with if observation came from a mountain site (often the case)
- Modelled CO (O3, Aerosol) concentrations have often large vertical gradients because of surface emissions
- Choosing the wrong level may leads to biases
- Methods for choosing the model levels
  1. Ignore mountain stations
  2. Difference between stations height and model orography
  3. Fit of simulated and observed meteorological parameters such as T or RH

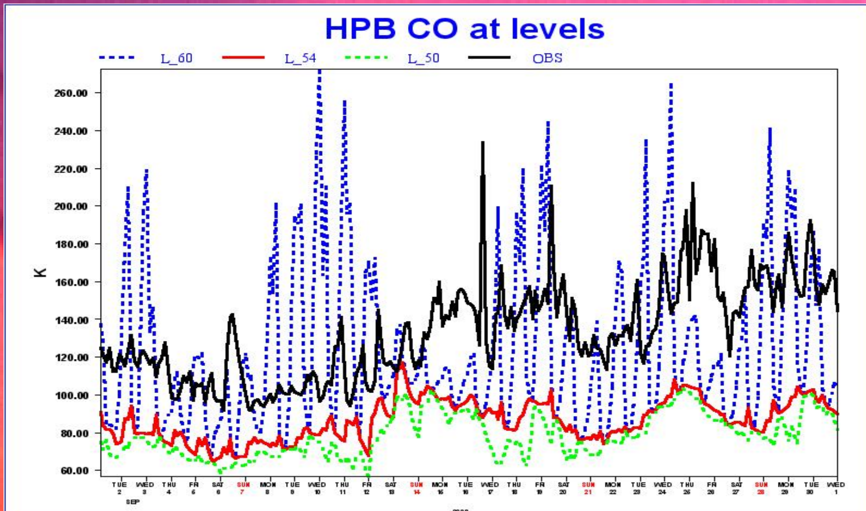
Example: Hohenpeissenberg – 980 m

- HPB is singular mountain close to the Alps
- Vertical modelled CO gradient in PBL (70%) and for ozone (-64 %)
- Difference between stations height and model orography

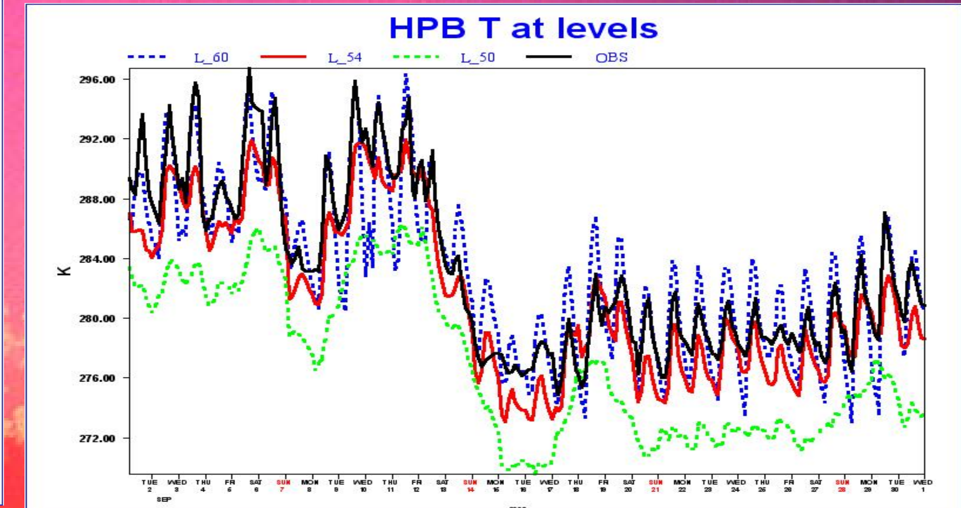
  125 km orography (GEMS) at HPB 1098 m -> level 60 (no mountain)

  16 km orography (vicinity of observation site) at HPB 575 m -> level 54 ("some"mountain)
- Choosing a small-scale orography seems to better indicate to what extent the observed air was influenced by surface processes

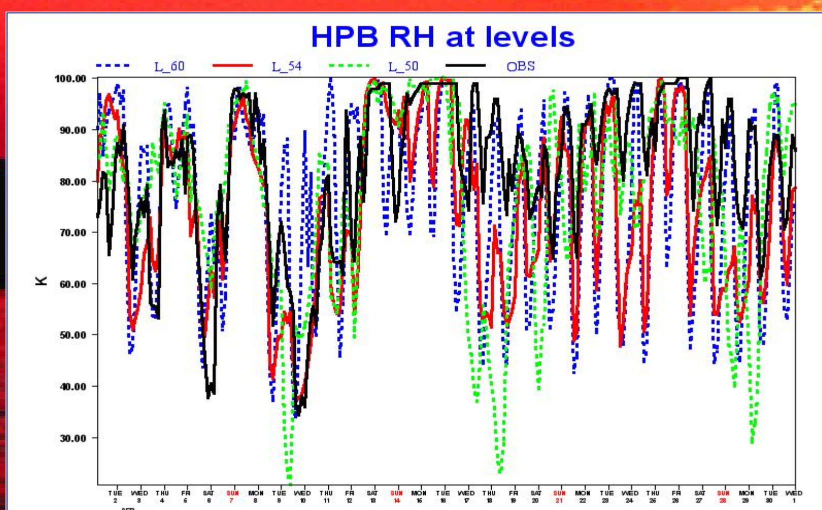
Modelled and observed CO for Level 50, 54 and 60 (September 2008)



- Large differences between levels 60 and 54
- Modelled surface diurnal cycle very strong
- Level 54 and 50 very similar



- Small differences for level 54 and 60 (in contrast to CO)
- Level 50 different from level 54
- 1st half of September: level 60 better fit
- 2nd half of September: level 54 better fit



Level 60 = 8m
Level 54 = 340 m
Level 50 = 950 m

… difficult to tell which level is best …

Sub-scale influence important!

Choosing the right model level for comparison with CO (O3) observations from GAW mountain stations (cont.)

- **Disregarding mountain observations is no good because there are so few observations and they sample tropospheric air**
- **Considering model orography vs. station height might be misleading for large-scale model (HPB would be below T159 surface)**
- **Considering high-resolution orography helps to better judge the close vicinity of the station**
- **Looking at T may confirm model level choice but T and CO profiles have a very different shape.**

Summary and requirements

- Validation has been proven fundamental for the future improvements of the GEMS analysis system.
- The strategy for the verification so far has involved the use of available independent satellite, ground and aircraft-based observations of chemical species.
- Several metrics to measure the quality of the analyses have been used

- Need reliable, readily available verifying data sets
- Consistency (same data set should be used for successive validations)
- Important to compare analysis and observations in the most objective way (see mountain site example)
- Realistic expectations from the assimilation (statistical process limited by assignment of background and observation errors and information content of the observations)
- Need to implement other diagnostics