Benefit of future S4-UVN and S5P ozone measurements: an ISOTROP STUDY

J.-L. Attié, W. Lahoz[1], S. Quesada-Ruiz, L. El Amraoui, P. Ricaud, R. Zbinden, H. Eskes, A. Segers, J. de Haan, J. Kujanpää, A. Oude Nijhuis, D. Schuettemeyer, J. Tamminen, R. Timmermans, P. Veefkind, and B. Veihelmann

[1]Presenter

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Outline

- Background
- ISOTROP OSSE setup, including tests of the setup
- Results – focus on ozone
- Conclusions

Background

ISOTROP:

Impact of Spaceborne Observations on Tropospheric Composition Analysis and Forecas

Objective:

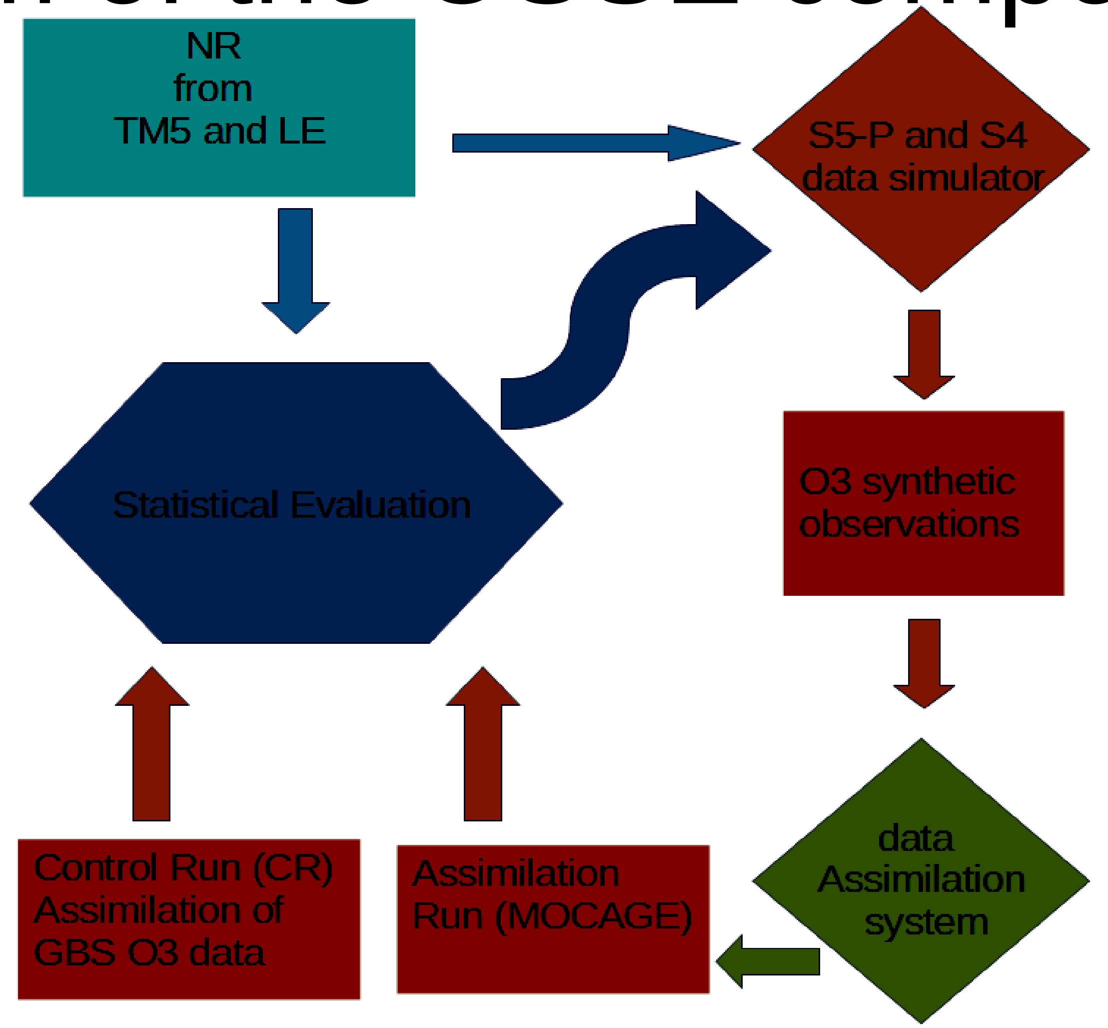
Quantify the benefit of the Sentinel 4, S4 (GEO) and Sentinel-5 Precursor, S5P (LEO) measurements of species such as ozone, CO, NO_2, HCHO
In particular vs ground-based observations and free model run
Focus on ozone in this presentation

Method:

Use OSSE (observing system simulation experiment) approach to quantify benefit

See Timmermans et al. (2015) for OSSEs concerning air quality measurements

OSSE Setup:
Diagram of the OSSE components



Cross-OSSE concept: TM5 and Lotos-Euros (LE) for Nature Run and use MOCAGE for DA
Avoid identical twin problem: avoid over-optimistic results (Masutani et al., 2010)

List of assimilation runs

Run ID	Run	Domain	Resolu-tion	Species	ASSIMILATION	
					GBS	Satellite
RREC	Free run	MACC	0.2°x0.2°	O3	no	no
RRLO (JJA)	LEO	MACC	0.2°x0.2°	O3	no	LE0/S5P O3
RRLGO (JJA)	OSSE,LEO +GEO	MACC	0.2°x0.2°	O3	no	LEO/S5P+ GEO/S4 O3
RRGO (JJA)	OSSE,GEO	MACC	0.2°x0.2°	O3	no	GEO/S4
RRLO	Reference	MACC Fire episode	0.2°x0.2°	O3	yes	no
ORELO	OSSE, LEO	MACC Fire episode	O.2°x0.2°	O3	yes	LEO/S5P O3
ORELGO	OSSE, LEO+GEO	MACC Fire episode	0.2°x0.2°	O3	yes	LEO/S5P+ GEO/S4 O3
OREGO	OSSE, GEO	MACC Fire episode	0.2°x0.2°	O3	yes	GEO/S4
OREGOC (June)	OSSE, GEO	MACC	0.2°x0.2°	O3	yes	Cloudy S4 pixels
ORELOC (June)	OSSE, LEO	MACC	0.2°x0.2°	O3	yes	Cloudy S5P pixels
OREGOR1 (June)	TEST R_obs=1	MACC	0.2°x0.2°	O3	no	GEO/S4

PERIOD:

SUMMER 2003 (JJA)

MACC DOMAIN:

15W – 35E
35N – 70N

Calculation of the Obs. Cov. Matrix for S4 and S5P

Calculation of the variance adapted to our DA system: $\boldsymbol{\sigma^2 = (A_t\, X_{NR} - X_r)^2}$

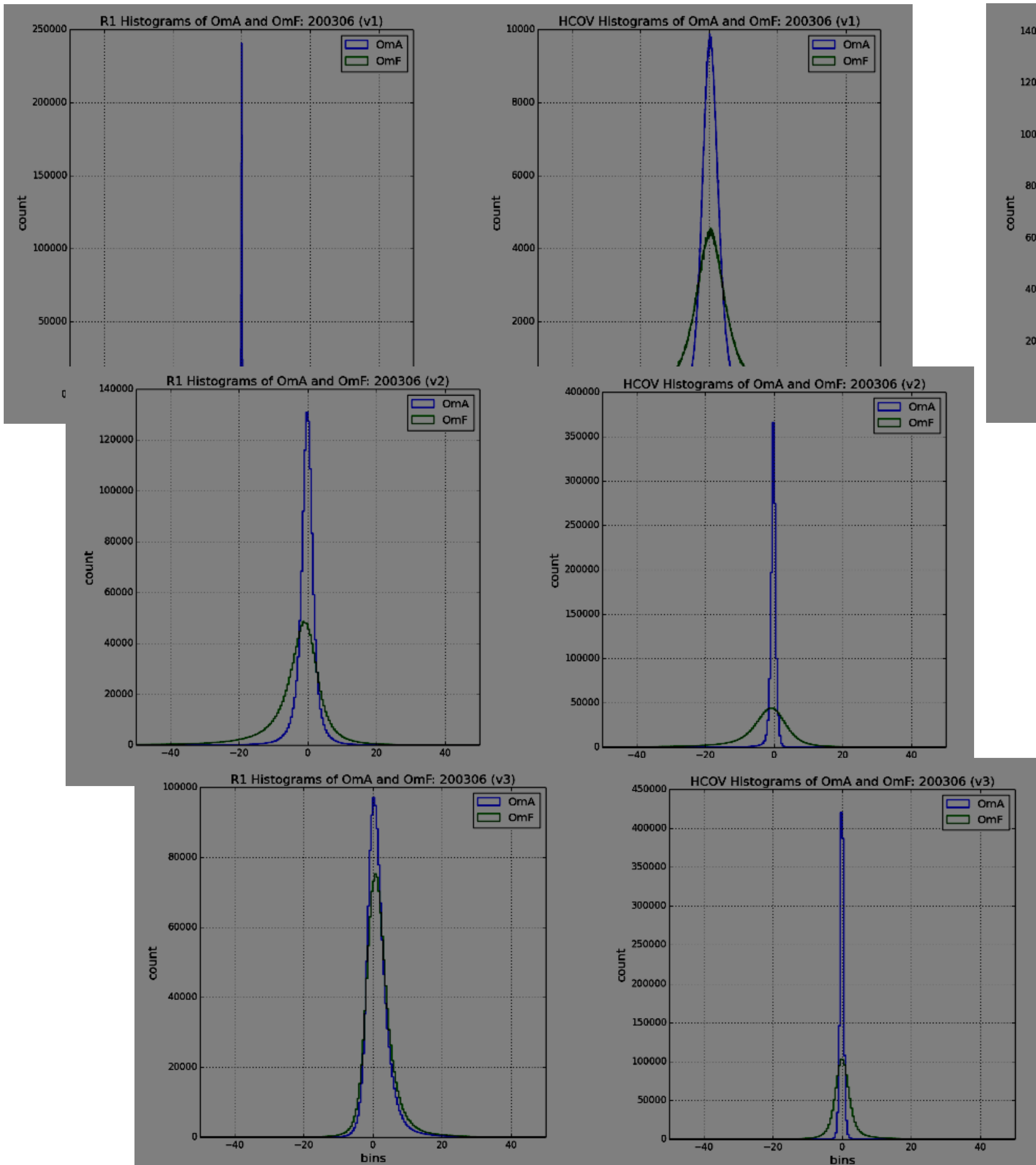
A_t: transformed AVK; X_{NR}: NR profile; X_r: ozone leading eigenvectors

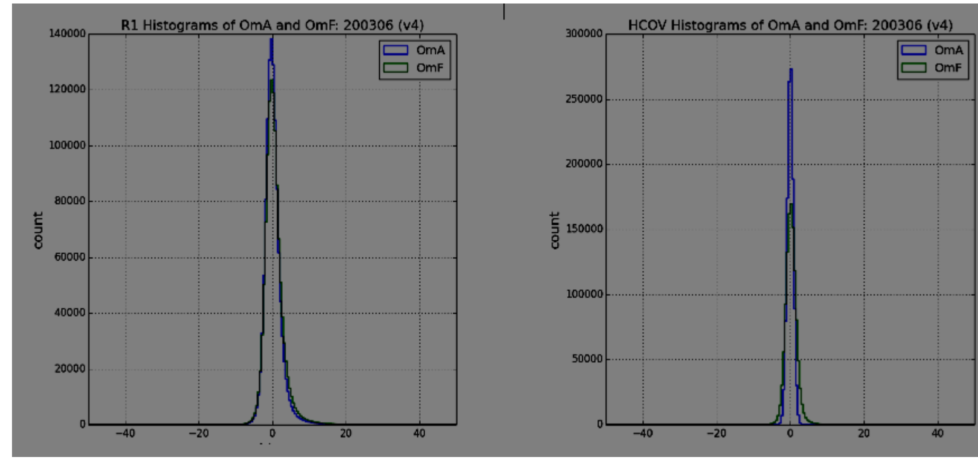
The Obs error cov matrix can be understood as : **RHCOV = R_obs + R_rep**

Retrieval stores 6 leading eigenvectors: 4-6 tropospheric information + some stratospheric information – values should be approx 1

Vector num	June		July		August		Nov		Dec		Jan	
Satellite	**S4**	**S5P**	**S4**	**S5P**	**S4**	**S5P**	**S4**	**S5P**	**S4**	**S5P**	**S4**	**S5P**
1	74.0	72.5	74.0	73.5	77.0	74.0	62.0	60.0	52.5	51.0	47.5	45.0
2	1.6	1.2	1.6	1.8	1.8	2.0	1.8	1.5	2.0	1.8	1.8	1.6
3	1.2	1.1	1.3	1.3	1.2	1.1	1.2	1.1	1.1	1.1	1.1	1.1
4	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
5	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
6	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0

OmA and OmF





This concerns the first 4 leading eigenvectors
using R_obs (KNMI & initial approach)
and R_HCOV (CNRM approach)

LH: ev1, ev2, ev3
RH: ev4
Panel: left (R_obs), right (HCOV)

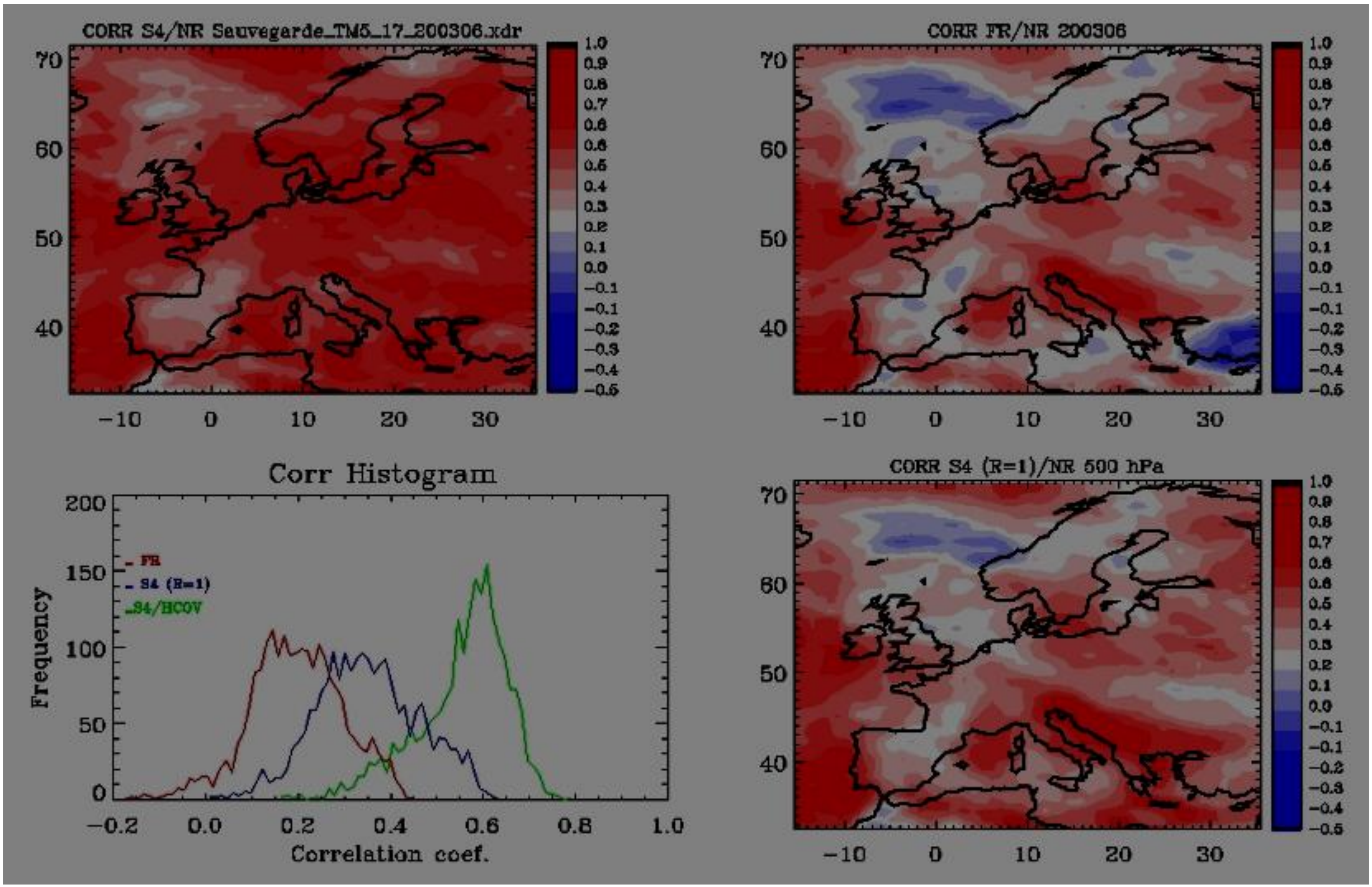
OmA narrower than OmF for all 4 evs for HCOV

Better representation of obs errors

Correlation using ROBS and RHCOV for June 2003 – 500 hPa

HCOV
S4 vs NR

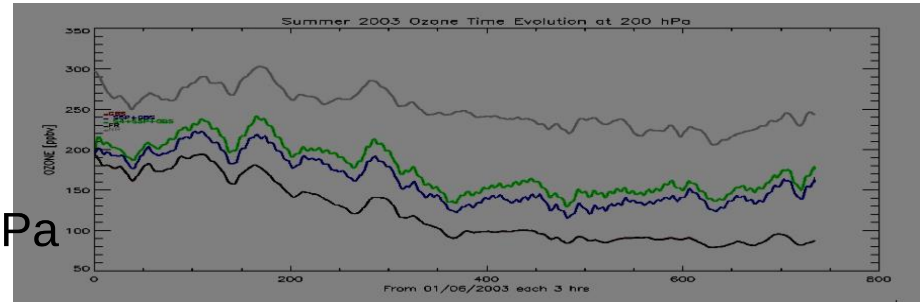
FR vs NR

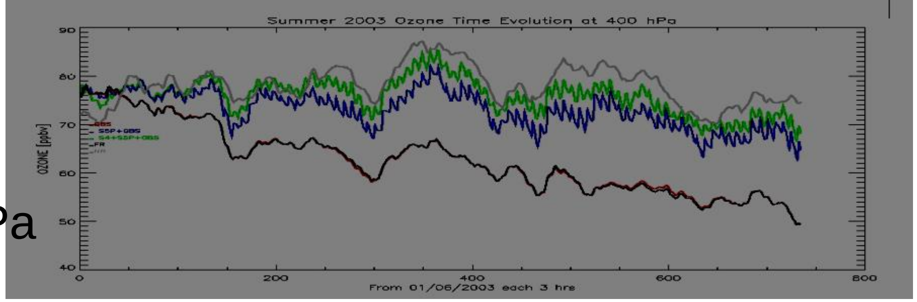


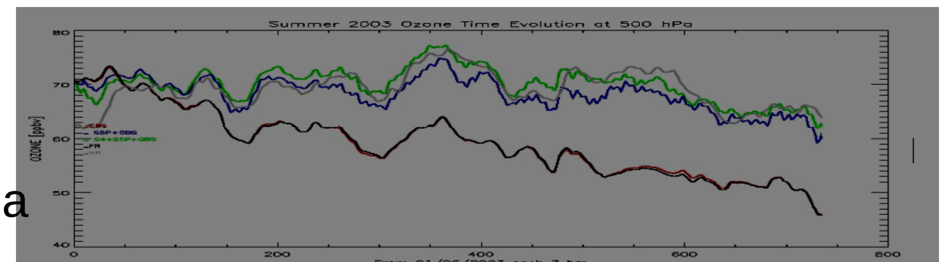
Histograms

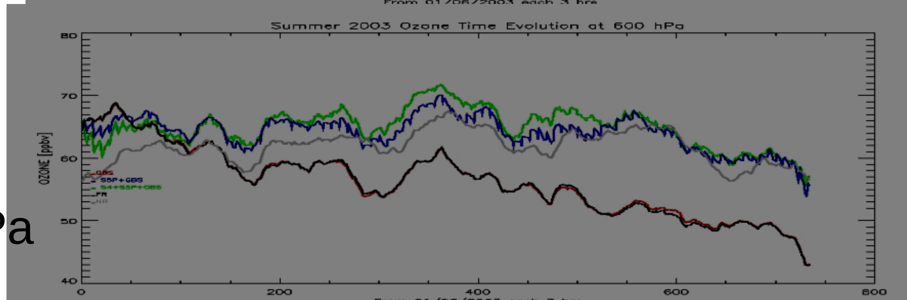
R=1
S4 vs NR

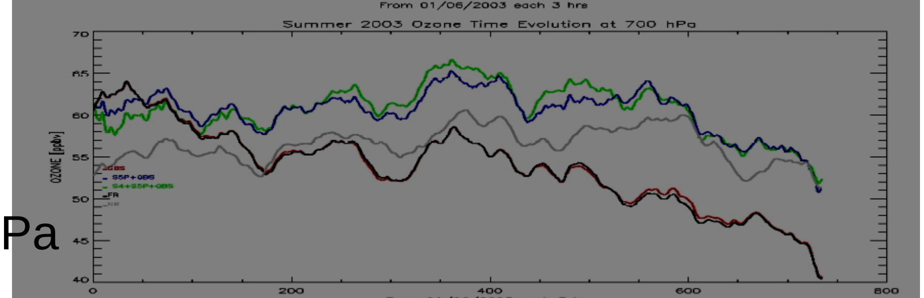
HCOV has a better representation of observation errors











Time-series of ozone for different pressure levels

Impact of different ozone observations

Free run: black
GBS DA: red
S5P+GBS: blue
S5P+S4+GBS: green
NR: grey

The AR are closer to the NR than the FR at 500 hPa and 600 hPa

500 hPa: S5P+S4+GBS better

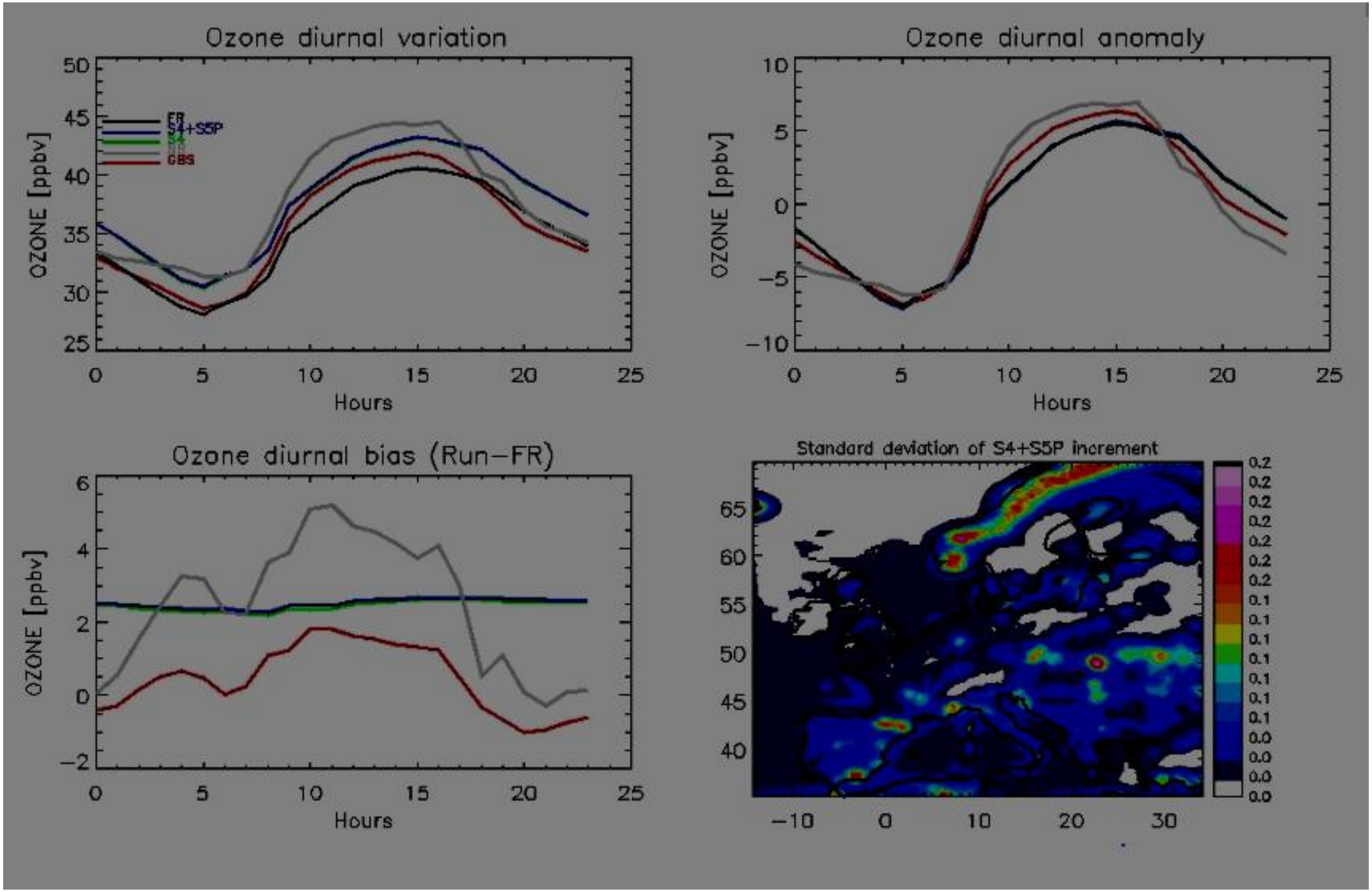
600 hPa: S5P+GBS (slightly better)

700 hPa: less impact from satellites; some impact from GBS

Diurnal variation at surface

FR: black
GBS: red
S5P+S4: blue
S4: green
NR: grey

No impact from S5P



Higher values in red

Results: the metrics used

$$\mathrm{MAE(X)} = \frac{1}{N}\sum |\mathrm{X} - \mathrm{NR}|;$$

Mean absolute error

$$\mathrm{RMSE(X)} = \sqrt{\frac{1}{N}\sum (\mathrm{X} - \mathrm{NR})^2};$$

Root mean square error

$$\mathrm{RMSERR(X)}=1- \frac{RMSE(AR)}{RMSE(RR)}$$

RMSE reduction rate or skill score

$$R(X) = \frac{\sum(X-\overline{X})(NR-\overline{NR})}{\sqrt{\sum(X-\overline{X})^2 \sum(NR-\overline{NR})^2}}$$

Correlation coefficient

Focus on ozone at 500 hPa and 700 hPa
Summer 2003 (JJA)

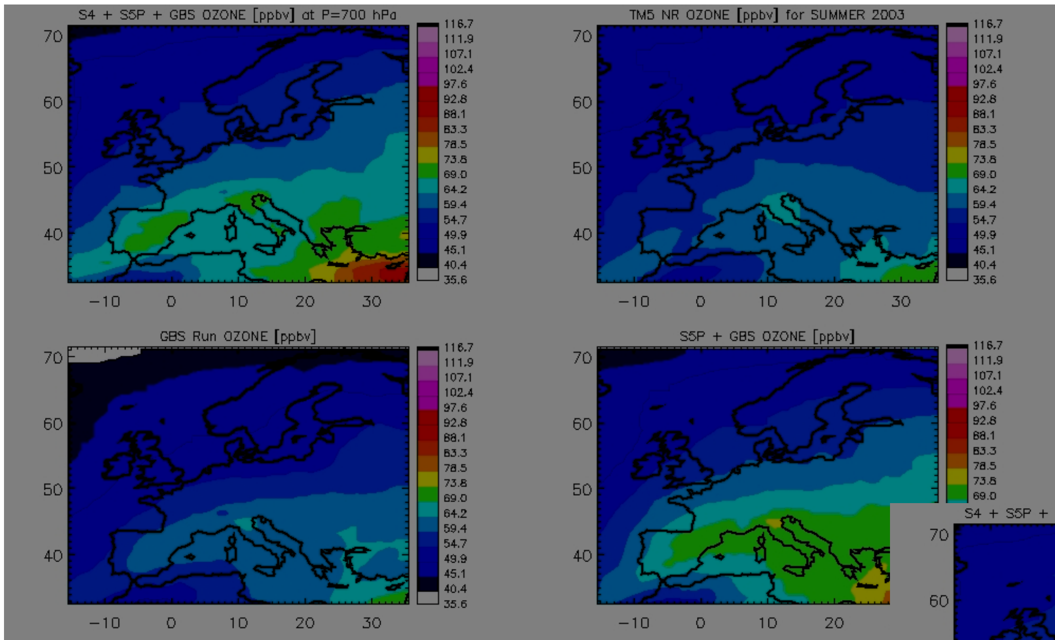
500 hPa and 700 hPa likely the low altitude limits where S4 and S5P can add values to our syster

→ No added value below 700 hPa

→ No clear added value at the surface

Ozone fields (ppbv) – summer 2003 (JJA)

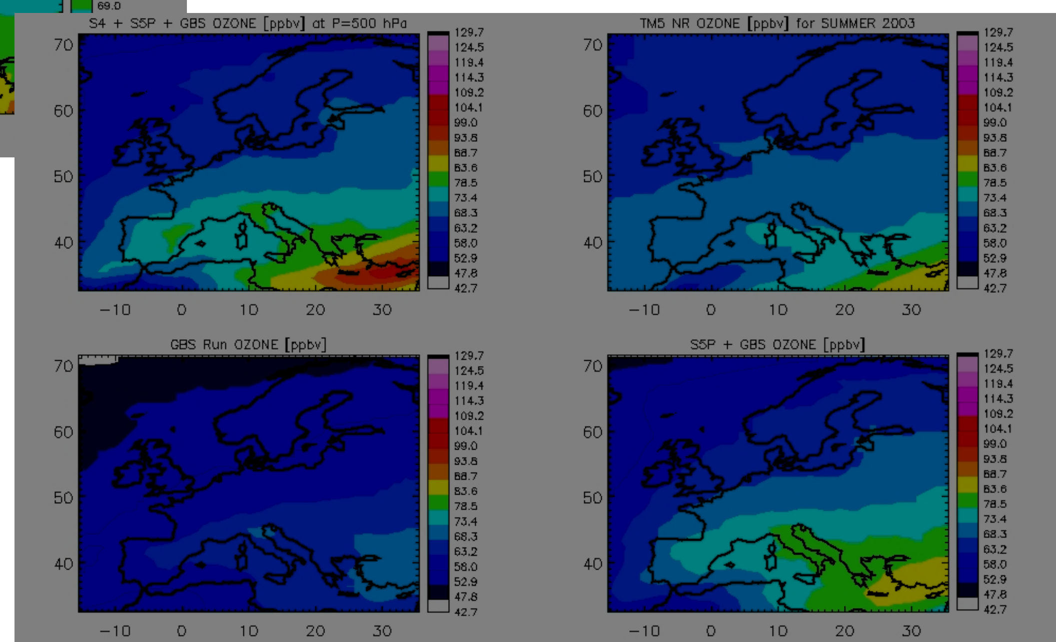
700 hPa



S4+S5P+GBS TM5 NR

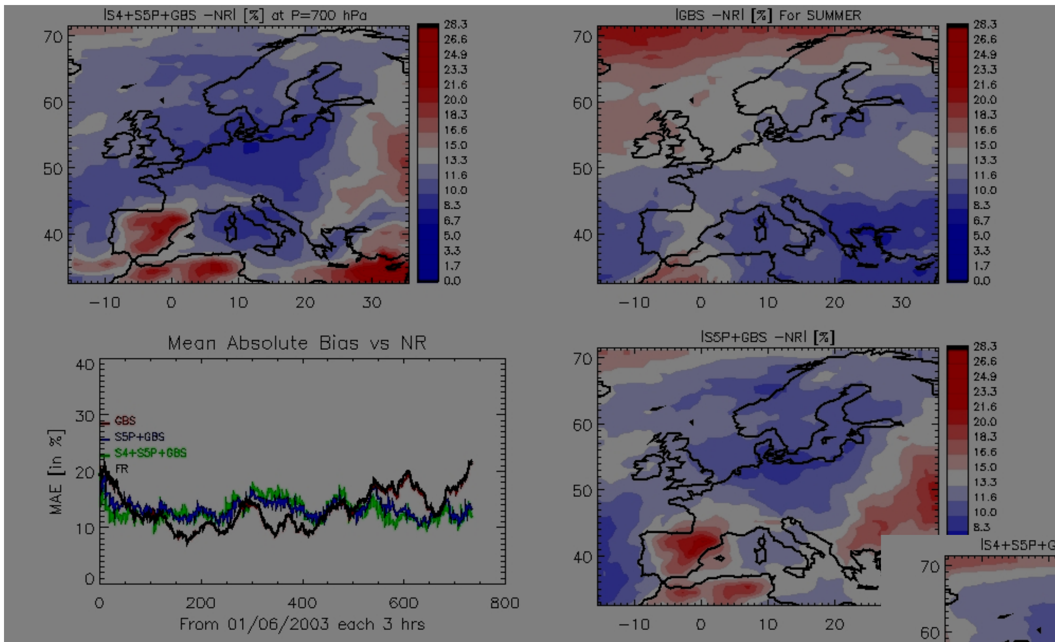
GBS S5P+GBS

500 hPa



MAE (%) – summer 2003 (JJA)

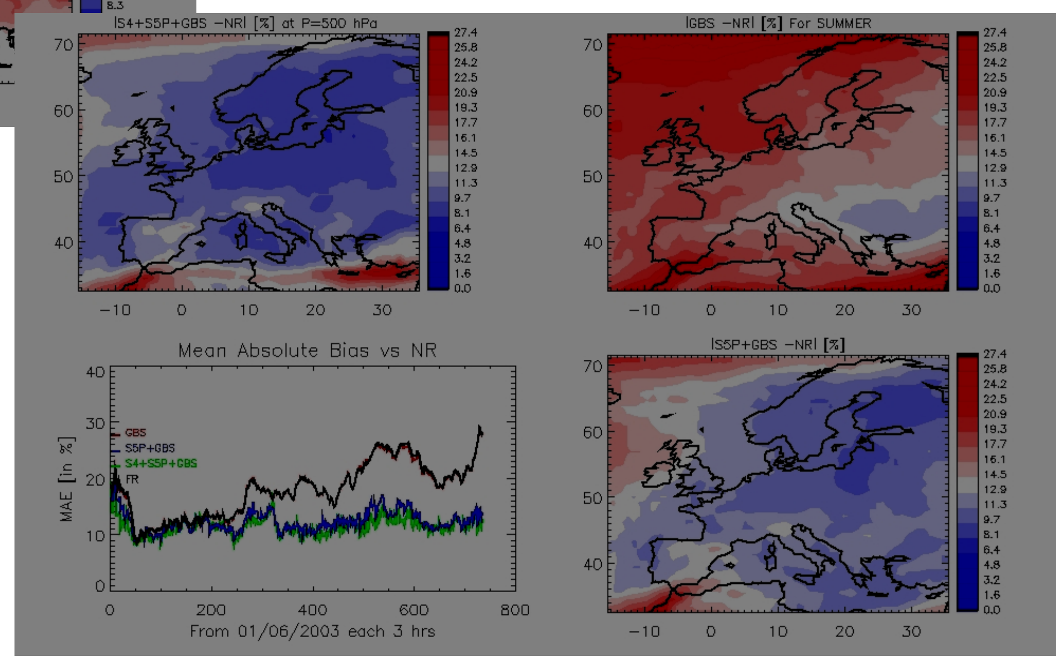
700 hPa



Abs(S4+S5P+GBS – NR) Abs(GBS – NR)

Mean abs bias vs NR Abs(S5P+GBS – NR)

500 hPa

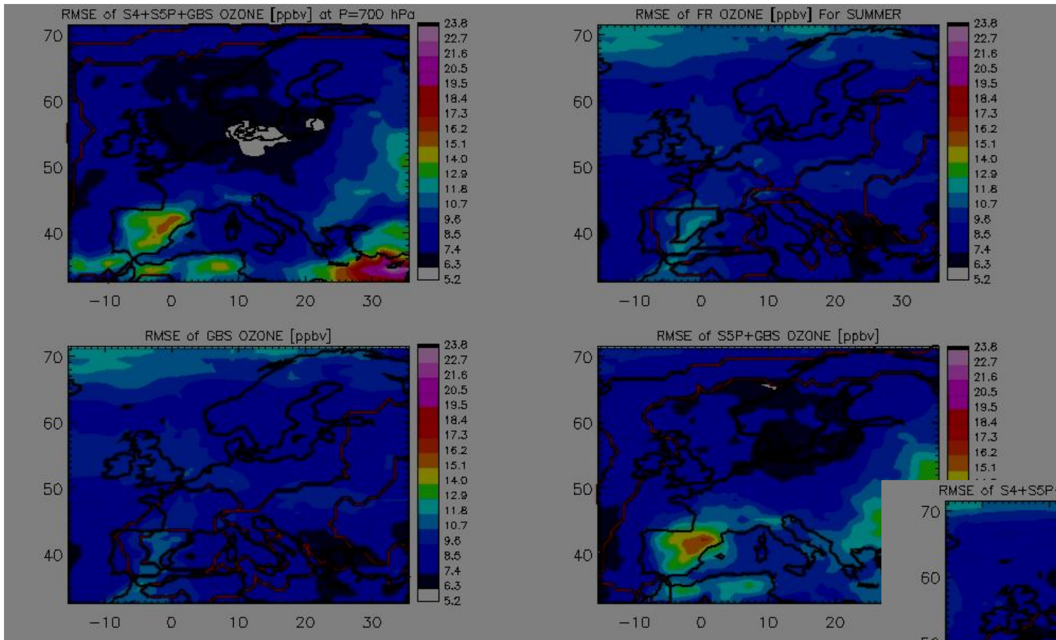


Some impact of S5P+S4 (not in S. Europe)

Impact of S5P+S4

RMSE (ppbv) – summer 2003 (JJA)

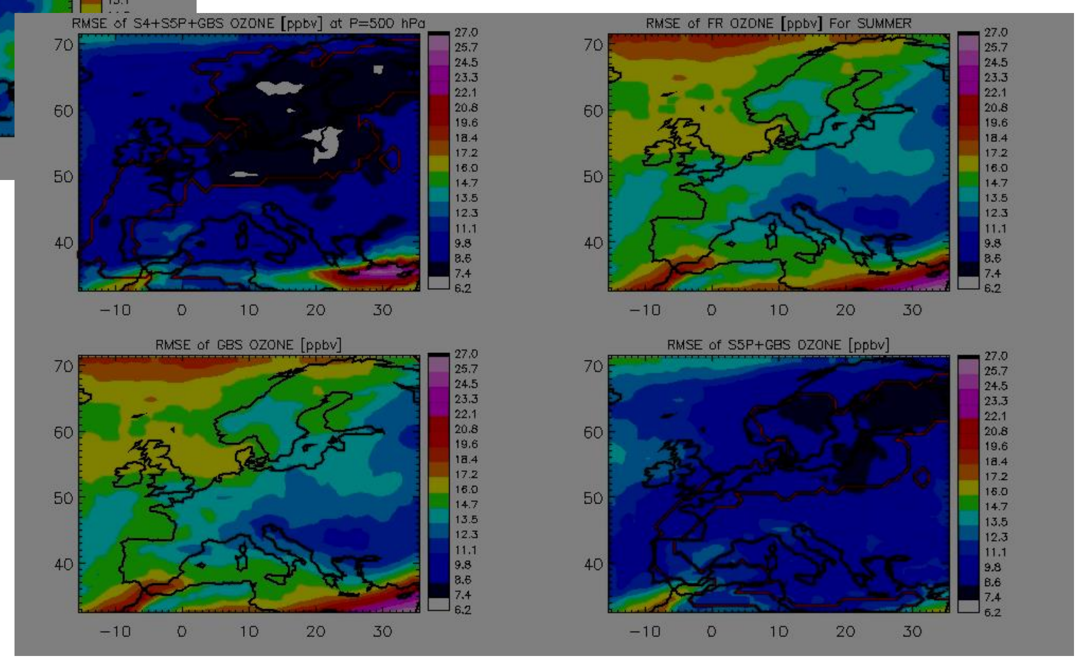
700 hPa



S4+S5P+GBS FR

GBS S5P+GBS

500 hPa

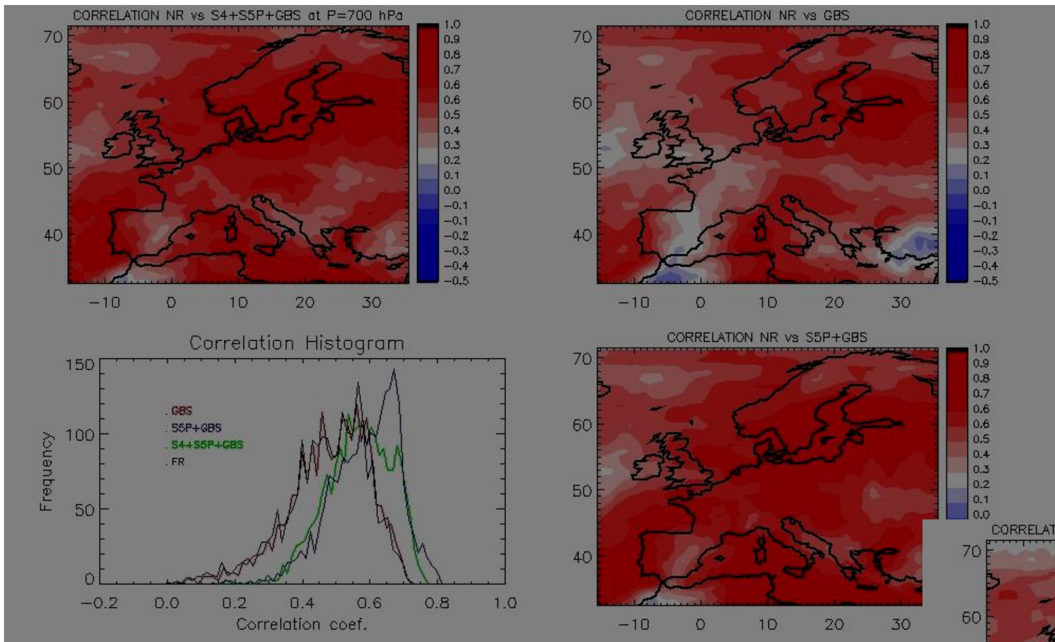


Some impact of S5P+S4
(not in S. Europe)

Impact of S5P+S4

Corr Coeff – summer 2003 (JJA) vs NR

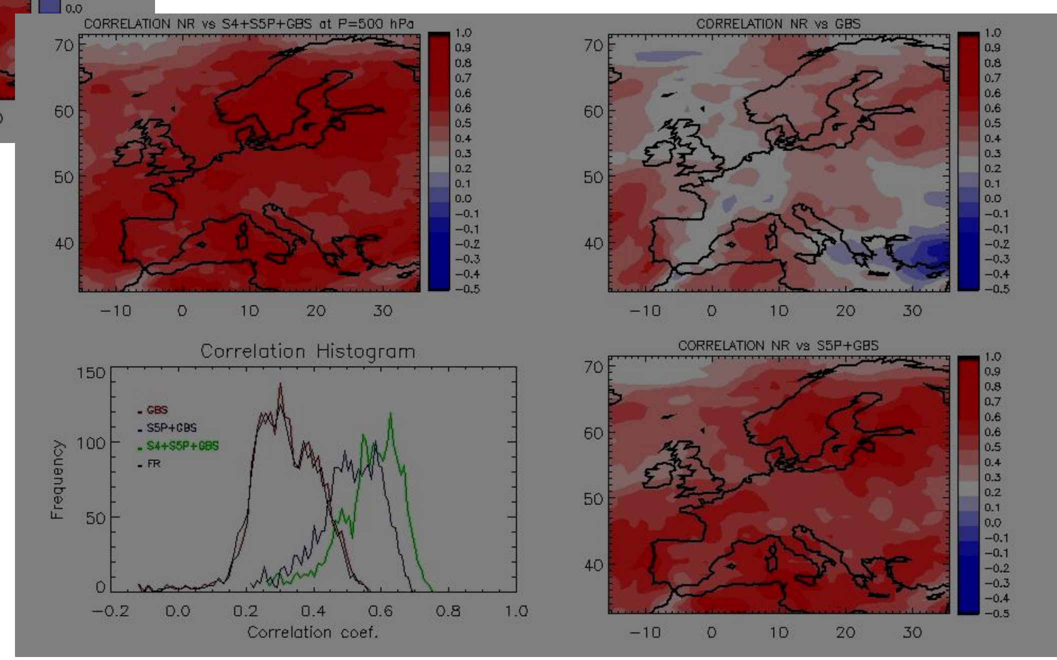
700 hPa



S4+S5P+GBS GBS

Histogram S5P+GBS

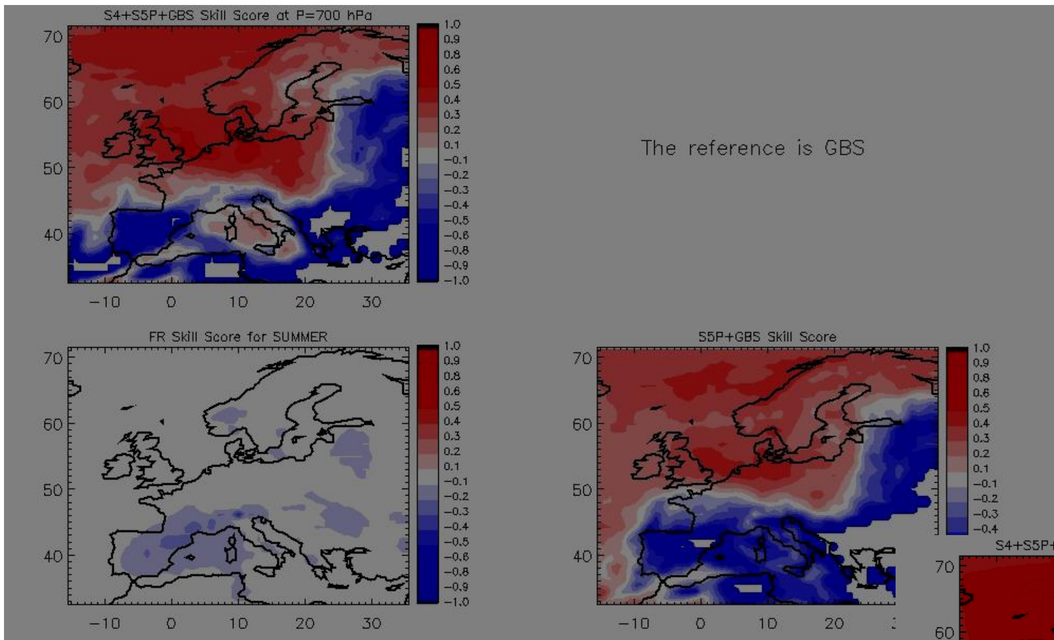
500 hPa



Impact of S5P+S4 →

Skill score summer 2003 (JJA) - ref is GBS

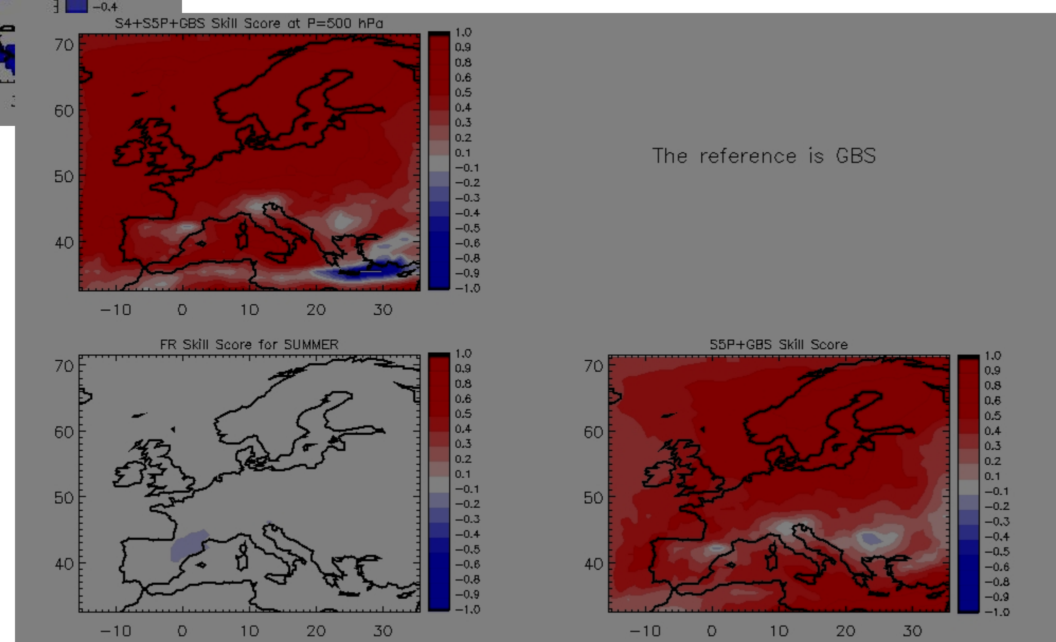
700 hPa



S4+S5P+GBS

FR S5P+GBS

500 hPa



S5P+S4 – impact vs FR

Some impact from S4

Conclusions

- *Some changes clearly visible in ozone field at 700 and 500 hPa with a slight increase of ozone in the SE part of the domain - closer to the NR than the RR (GBS)*
- *Main improvement is stabilization and decrease of bias (vs NR) over the period (Summer 2003 – JJA) of about 10 % at 700 hPa and 30% instead of 60% at 500 hPa. Impact is similar for S5P and S4+S5P with slightly better performance for the double assimilation (S4+S5P)*
- *AR of S4 and S5P show more variability than the RR and the FR at 700 hPa whereas they show slightly less variability at 500 hPa - Except for S4+S5P assimilation where more variability is visible in the SE part of the domain comparable to the RR and FR*
- *Improvement for both levels in the correlation (vs NR) when we add S4 or S5P. The histogram is slightly improved at 700 hPa whereas at 500 hPa it goes from 0.3 (GBS or RR) to 0.5 (S5P) and 0.5 (S4+S5P)*
- *For both levels (700 hPa, 500 hPa), there is net improvement in the domain in terms of skill score with values closer to 1 for the double assimilation except in the SE of the domain*
- *Benefit from S4 and S5P ozone at 500 hPa and 700 hPa – see MAGEAQ presentation*