



**Barcelona
Supercomputing
Center**

Centro Nacional de Supercomputación

CALIOPE forecasts evaluated by DELTA

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Valentina Sicardi, Kim Serradell, and CALIOPE team

**WG1 Assessment – CCA: Forecast
FAIRMODE Technical Meeting . April 28-29, 2014. Kjeller (Norway)**

CALIOPE Air Quality Forecast System

CALIOPE modules

Meteorology

- WRF-ARWv3.5
- 38 sigma levels (top 50 hPa)
- IBC: GFS (NCEP)
- 33 layers/50 hPa

Emission

- HERMESv2
- EU: HERMES-DIS (EMEP data)
- Spain: HERMES-BOUP

Chemistry

- CMAQv5.0.1
- CB05/AERO5
- BC: NCAR MOZART4
- 15 layers/ 50 hPa

Desert dust

- BSC-DREAM8bv2
- Desert PM10 and PM2.5

Post-process

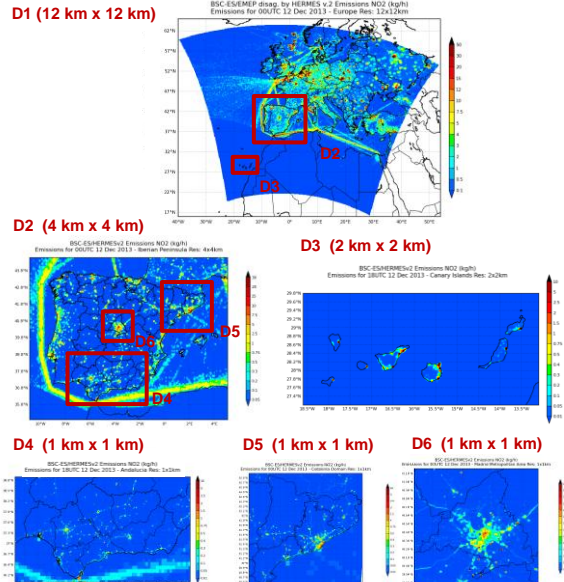
- Kalman filter (point and 2D)

Air Quality Forecast

O₃, NO₂, SO₂, CO, PM10, PM2.5, Benceno

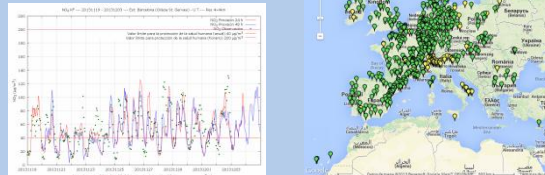
Forecast 48h

- Maps: concentración, emission, meteo.
- Air Quality Index



NRT evaluation

- AQ and Met network
- Satellites



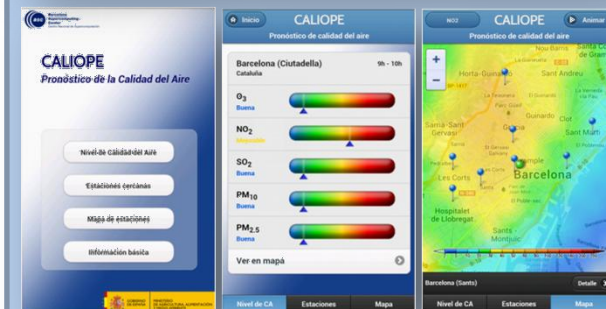
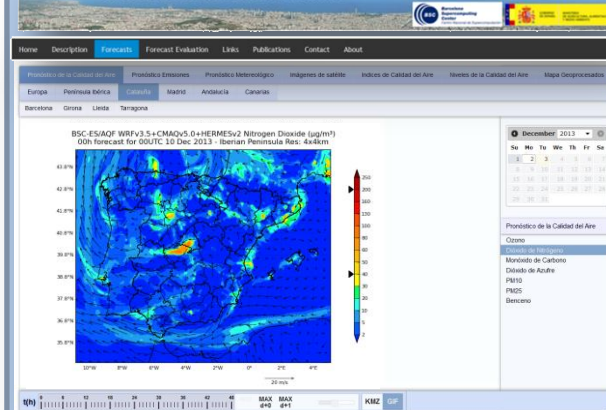
Difusion

- Web (www.bsc.es/caliope)
- Smartphone



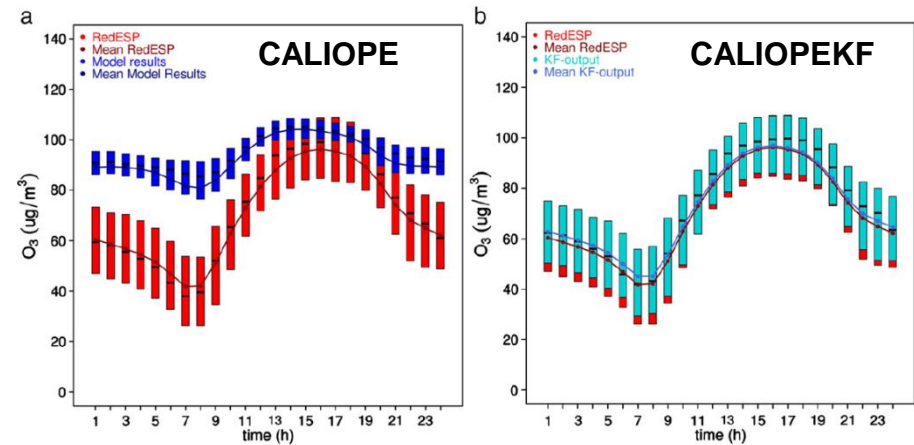
Sistema CALIOPE

Pronóstico de la Calidad del Aire

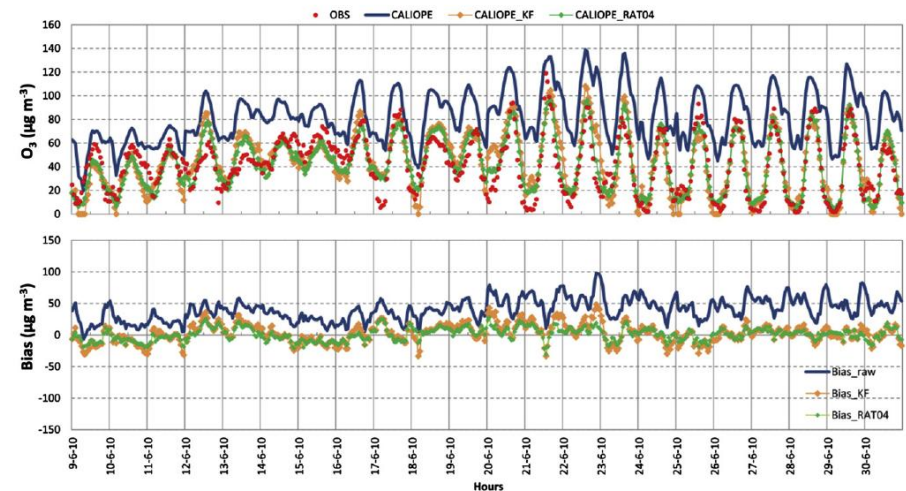


Experience with bias-correction techniques in CALIOPE

- ❧ KF improves O₃ forecast (timing, daily variability) bias and capability to predict exceedances of air quality thresholds.
- ❧ Among different bias-correction techniques, KF was more robust in terms of the absence of observation and computational cost.
- ❧ KF is applied for O₃, NO₂, and PM₁₀



Sicardi et al. (2011): STOTEN- Assessment of Kalman filter bias-adjustment technique to improve the simulation of ground-level ozone over Spain



Borrego et al. (2011): AE- How bias-correction can improve air quality forecasts over Portugal

Objective

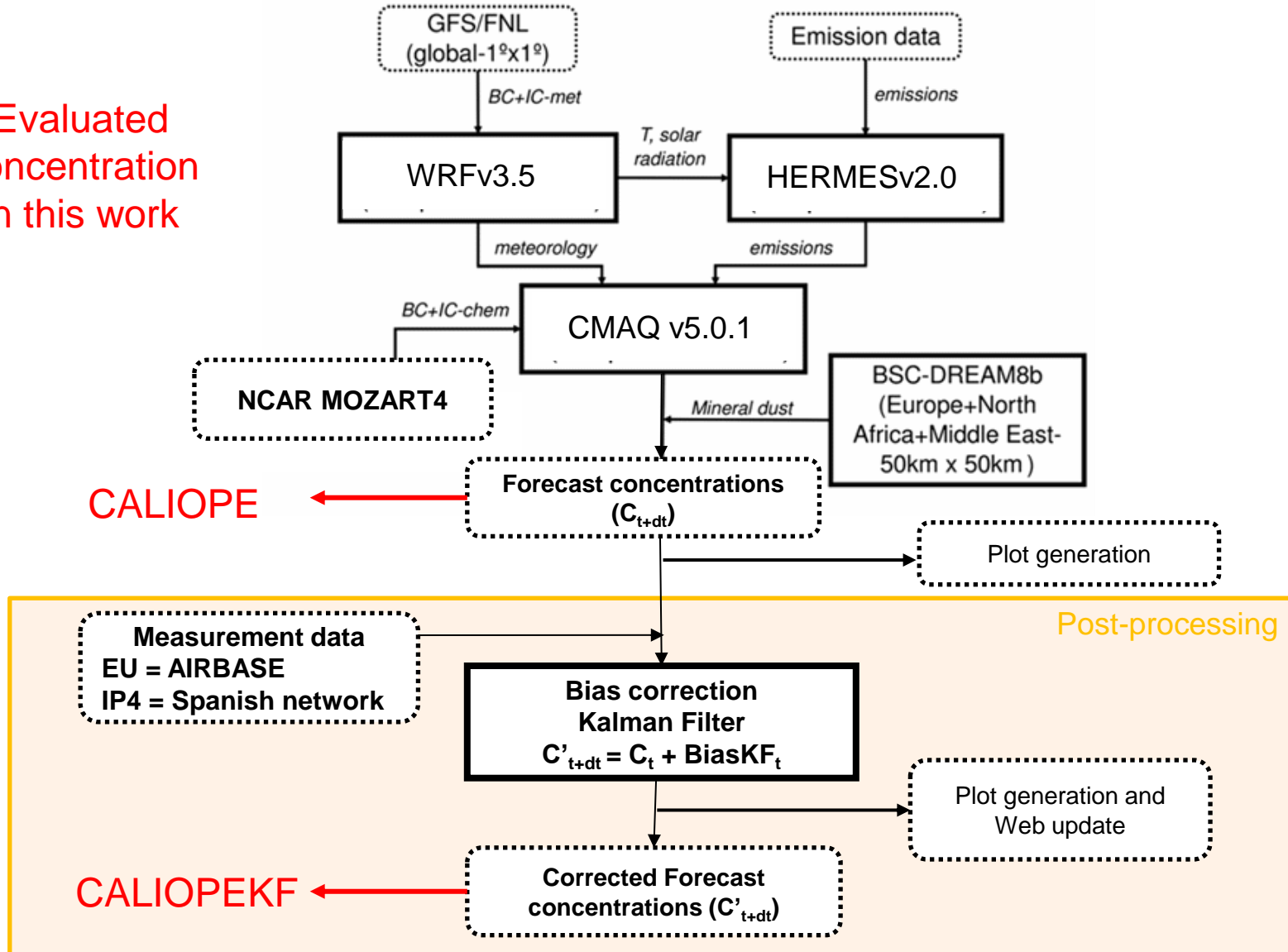
- Using the DELTA tool (benchmarking and exploration) to evaluate the CALIOPE performance, with a special focus on:
 - Analysing the effect of bias correction techniques in terms of the MQO.
 - Testing the Target Indicator for forecasting applications.

Case study

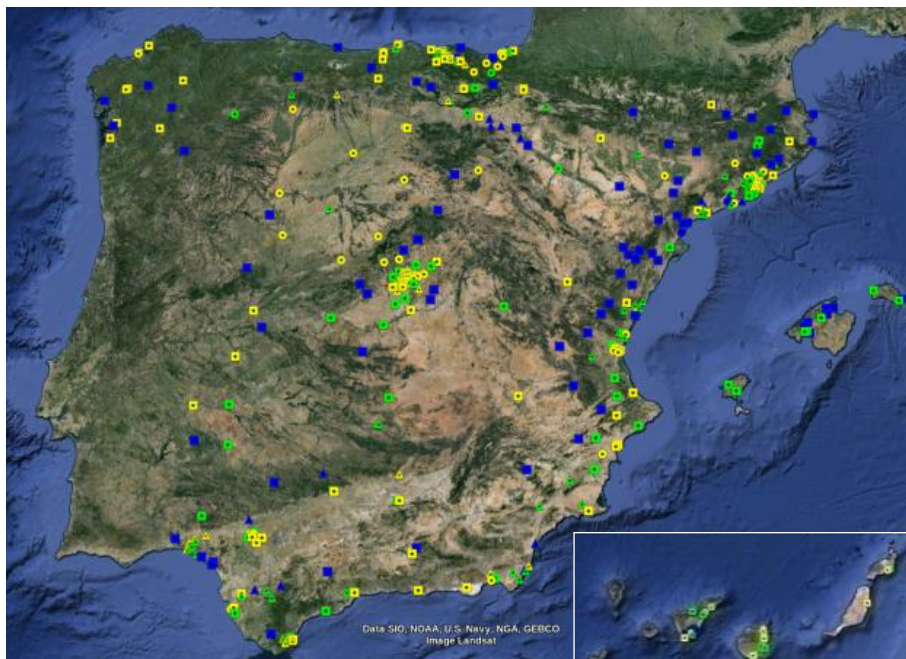
- **Modelling system:** CALIOPE-AQFS (4 km x 4 km)
- **Domain:** Spain
- **Annual evaluation:** 2013
- **Evaluated pollutants:** O₃ and NO₂
- **Observation:** Spanish air quality monitoring network.
- **DELTA tool v3.6:**
init.ini: ELAB_FILTER_TYPE=ADVANCED

Forecast **post-processing** within CALIOPE-AQFS

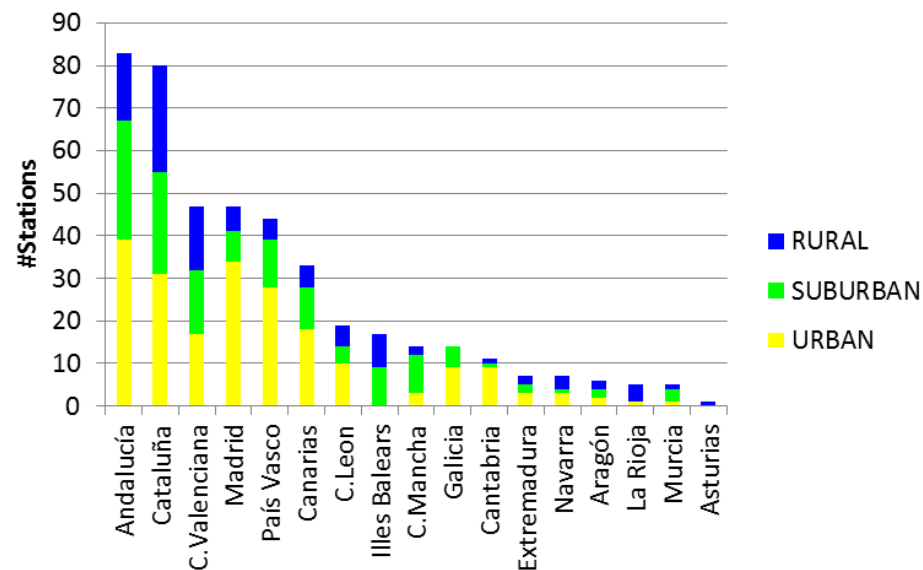
Evaluated concentration in this work



AQ Monitoring Network in 2013: Near Real Time (NRT) observations



445 stations = 117 Rural – 127 Suburban – 201 urban



Institutions providing data in NRT during 2013:

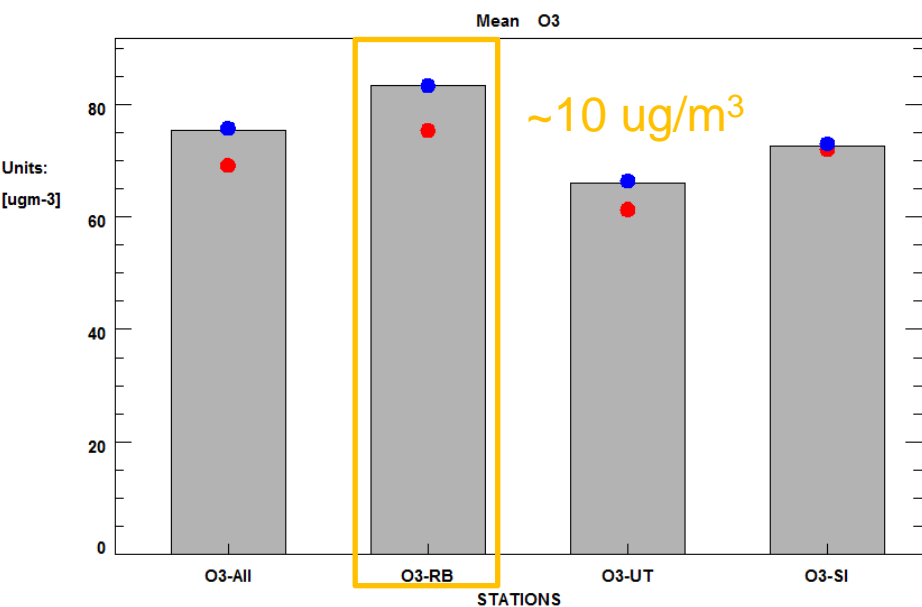
1. La Agencia Europea de Medioambiente (EEA)
2. [Generalitat de Catalunya](#)
3. [Gobierno de Cantabria](#)
4. [Junta de Andalucía](#)
5. [Gobierno de Canarias](#)
6. [Comunidad de Madrid](#)
7. [Ayuntamiento de Madrid](#)
8. [Govern de les Illes Balears](#)
9. [Xunta de Galicia](#)
10. [Gobierno de La Rioja](#)
11. [Gobierno Extremadura](#)
12. [Junta de Castilla y León](#)
13. [Junta de Castilla-La Mancha](#)
14. [Govern d'Andorra](#)

	# stations	%U	%S	%R
O ₃	290	42	30	29
NO ₂	345	48	29	23
SO ₂	250	48	29	20
PM10	223	51	29	20
PM2.5	43	42	33	26

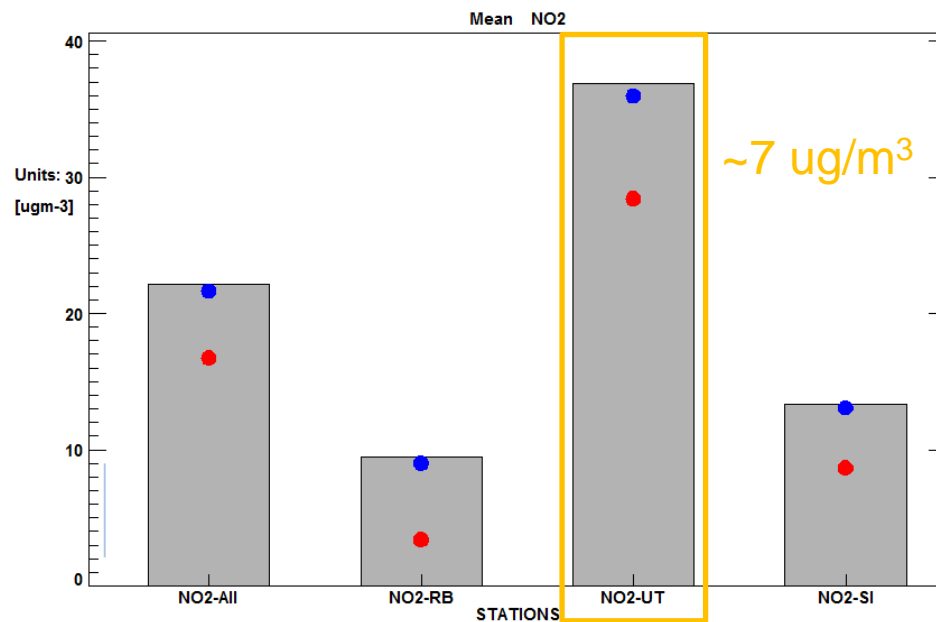
Bar plot in DELTA tool

● CALIOPE
● CALIOPEKF

O₃



NO₂



● CALIOPE
● CALIOPEKF

□ OBS

O₃ period
(April to September)

Str/End Ind: 2161-5832
Station: -1
Parameter: O3
Scen: 2013
Extra Values: No
Season: Year
Day hours: All 24h
Time Average: Preserved
Daily stats: preserved

● CALIOPE
● CALIOPEKF

□ OBS

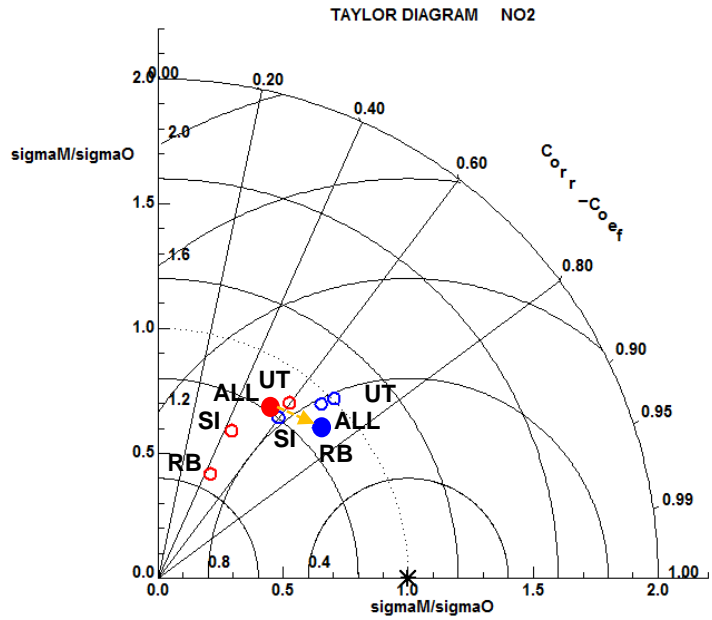
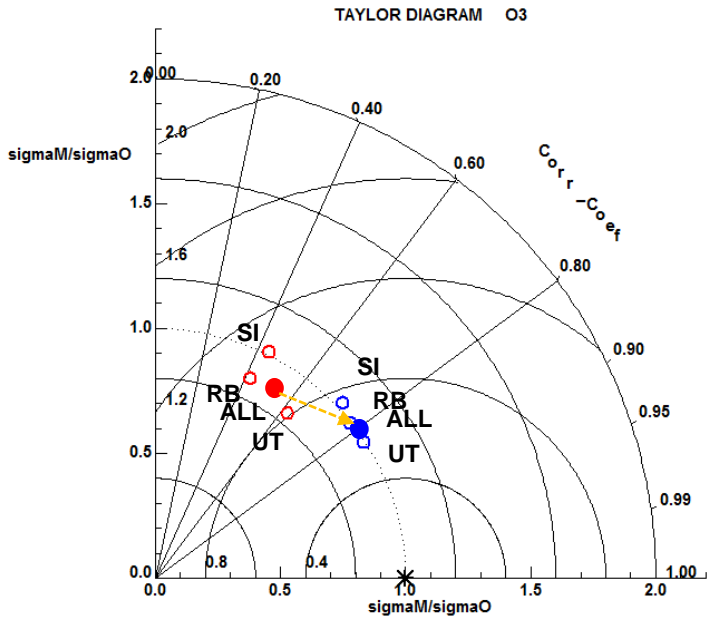
Str/End Ind: 1-8760
Station: -1
Parameter: NO2
Scen: 2013
Extra Values: No
Season: Year
Day hours: All 24h
Time Average: Preserved
Daily stats: preserved

Taylor diagram in DELTA tool

● CALIOPE
● CALIOPEKF

O₃

NO₂



● CALIOPE
● CALIOPEKF

Str/end Ind: 1-8760
 Station: -1
 Parameter: O3
 Scen: 2013
 Extra Values: No
 Season: Year
 Day hours: All 24h
 Time Average: Preserved
 Daily stats: Mean

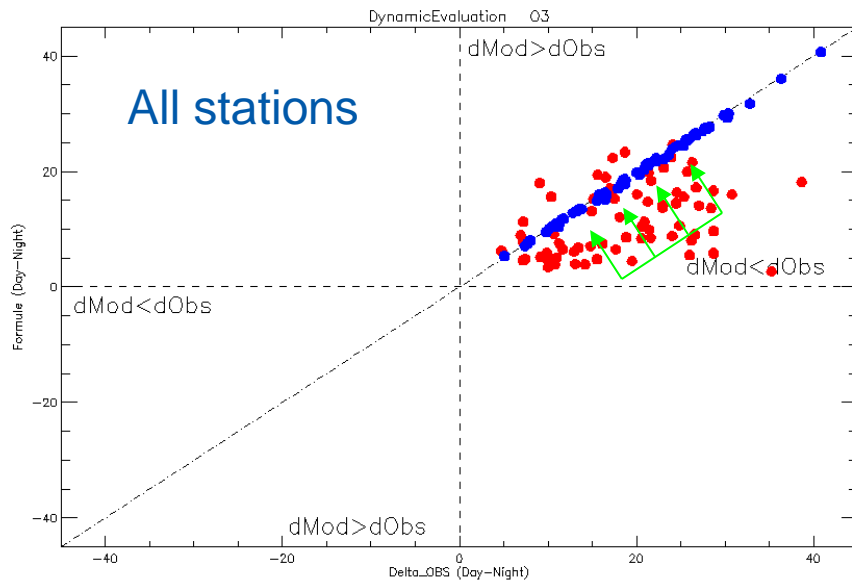
● CALIOPE
● CALIOPEKF

Str/end Ind: 1-8760
 Station: -1
 Parameter: NO2
 Scen: 2013
 Extra Values: No
 Season: Year
 Day hours: All 24h
 Time Average: Preserved
 Daily stats: Mean

Dynamic evaluation: day/night

• CALIOPE
• CALIOPEKF

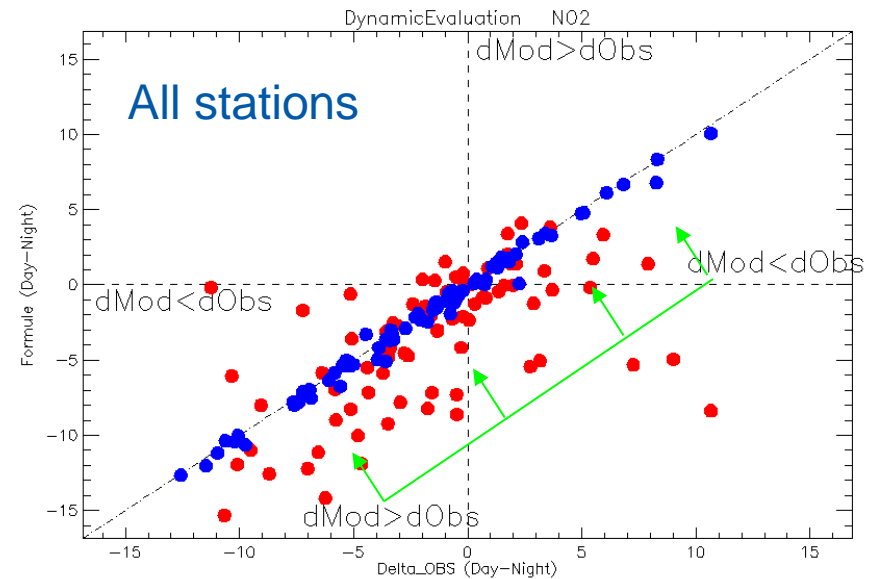
O₃



• CALIOPE
• CALIOPEKF

Str/End Ind: 1-8760
 Parameter: O3
 Scen: 2013
 Extra Values: No
 Season: Year
 Day hours: Day-Night
 Time Average: Preserved
 Daily stats: preserved

NO₂

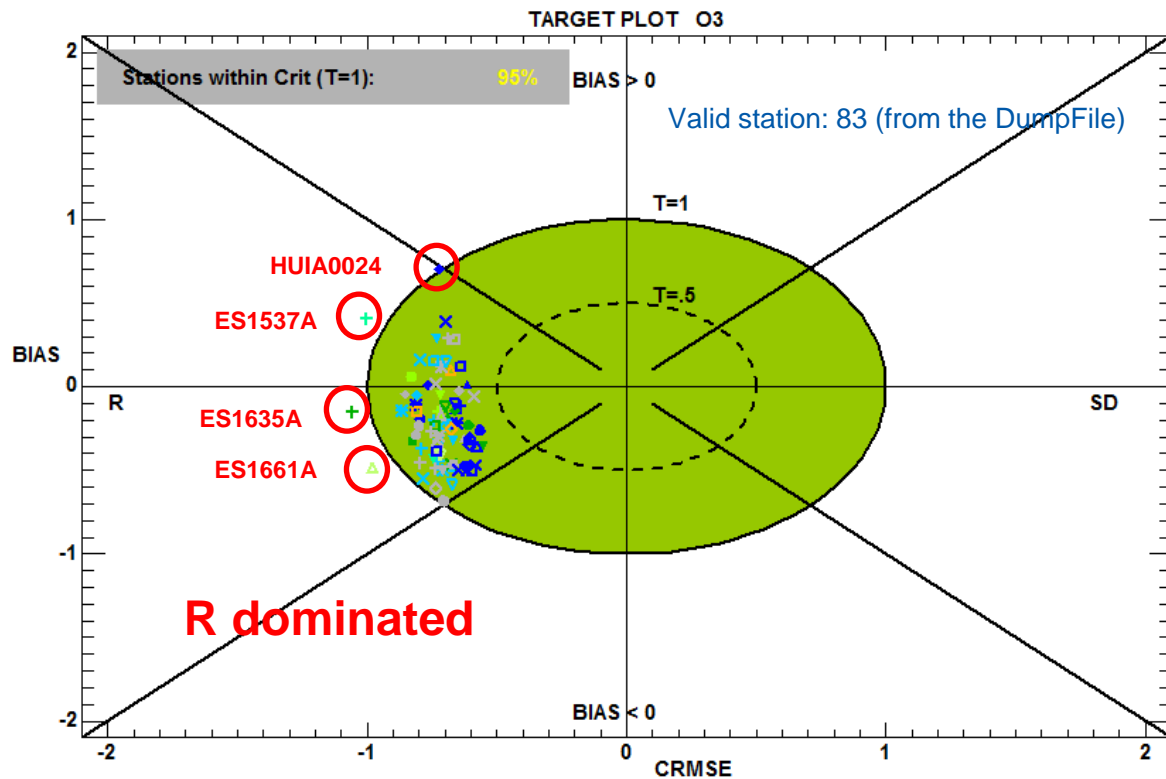


• CALIOPE
• CALIOPEKF

Str/End Ind: 1-8760
 Parameter: NO2
 Scen: 2013
 Extra Values: No
 Season: Year
 Day hours: Day-Night
 Time Average: Preserved
 Daily stats: preserved

Day-night variability (almost negative) is significantly improved with KF

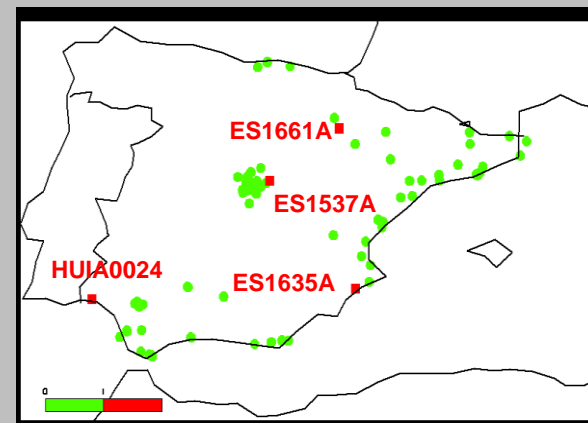
Target Plot and GeoMap



From Target plot description in User

$$\frac{\text{NMSD}}{\sqrt{2(1-R)}} \begin{cases} > 1 \rightarrow \text{SD dominates on R (left)} \\ < 1 \rightarrow \text{R dominates on SD (right)} \end{cases}$$

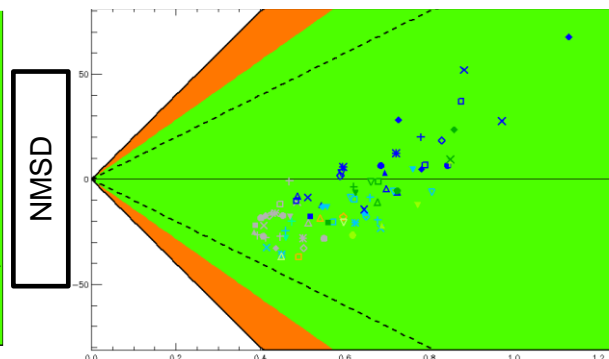
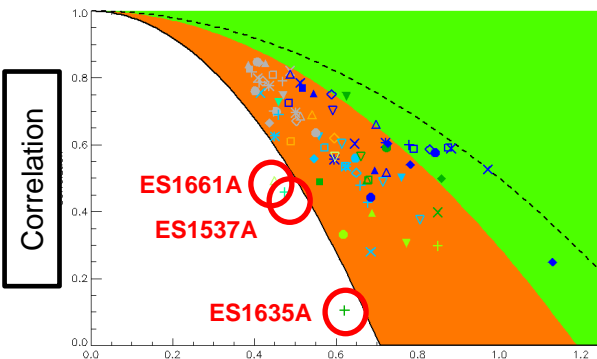
GeoMap (Target)



- Criterion <= 1
- Bias >= 0
- Bias < 0
- △ R dominated
- Sigma dominated

Stated ind: 1.8760
Model (s): CALIOPE
Parameter: O3
Score: 2012
Extra Values: No
Season: Year
Day hours: All 24h
Time Average: 8h
Daily stats: Max

It is not consistent

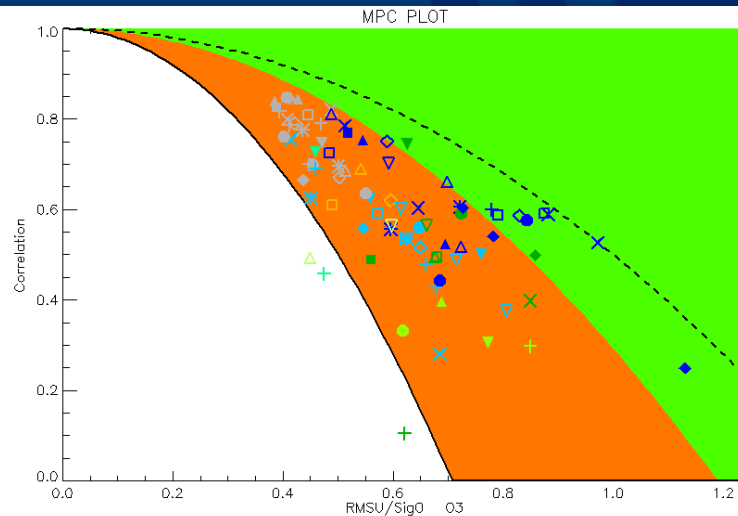
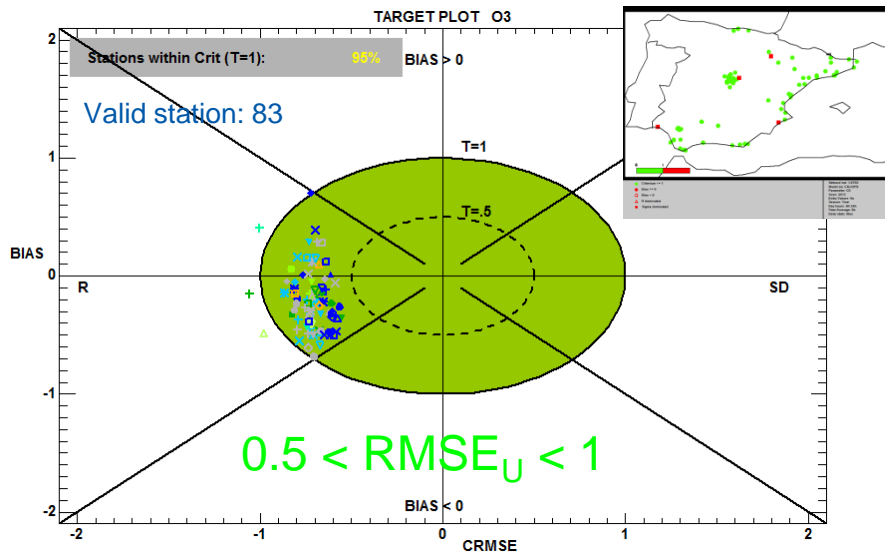


A3	AY	CAIA25	ES1192A	ES1192A	ES1192A
AA	AZ	CAIA26	ES1386A	ES1386A	ES1386A
AL	BA	CAIA27	ES1400A	ES1400A	ES1400A
ALIA0011	BB	CAIA28	ES1417A	ES1417A	ES1417A
ALIA0012	BC	CAIA29			
ALIA0018	BD	CAIA30			
ALIA0021	BE	CAIA31			
BM	BF	CAIA32			
CAIA0210	BG	CAIA33			
CAIA0219	BH	CAIA34			
CAIA2529	BI	CAIA35			
	BJ	CAIA36			
	BK	CAIA37			
	BL	CAIA38			
	BM	CAIA39			
	BN	CAIA40			
	BO	CAIA41			
	BP	CAIA42			
	BQ	CAIA43			
	BR	CAIA44			
	BS	CAIA45			
	BT	CAIA46			
	BU	CAIA47			
	BV	CAIA48			
	BW	CAIA49			
	BX	CAIA50			
	BY	CAIA51			
	BZ	CAIA52			
	CA	CAIA53			
	CB	CAIA54			
	CC	CAIA55			
	CD	CAIA56			
	CE	CAIA57			
	CF	CAIA58			
	CG	CAIA59			
	CH	CAIA60			
	CI	CAIA61			
	CJ	CAIA62			
	CK	CAIA63			
	CL	CAIA64			
	CM	CAIA65			
	CN	CAIA66			
	CO	CAIA67			
	CP	CAIA68			
	CQ	CAIA69			
	CR	CAIA70			
	CS	CAIA71			
	CT	CAIA72			
	CU	CAIA73			
	CV	CAIA74			
	AW	CAIA75			
	AX	CAIA76			
	AY	CAIA77			
	AZ	CAIA78			
	AA	CAIA79			
	AB	CAIA80			
	AC	CAIA81			
	AD	CAIA82			
	AE	CAIA83			
	AF	CAIA84			
	AG	CAIA85			
	AH	CAIA86			
	AI	CAIA87			
	AJ	CAIA88			
	AK	CAIA89			
	AL	CAIA90			
	AM	CAIA91			
	AN	CAIA92			
	AO	CAIA93			
	AP	CAIA94			
	AQ	CAIA95			
	AR	CAIA96			
	AS	CAIA97			
	AT	CAIA98			
	AU	CAIA99			
	AV	CAIA00			

A3	AY	CAIA25	ES1192A	ES1192A	ES1192A
AA	AZ	CAIA26	ES1386A	ES1386A	ES1386A
AL	BA	CAIA27	ES1400A	ES1400A	ES1400A
ALIA0011	BB	CAIA28	ES1417A	ES1417A	ES1417A
ALIA0012	BC	CAIA29			
ALIA0018	BD	CAIA30			
ALIA0021	BE	CAIA31			
BM	BF	CAIA32			
CAIA0210	BG	CAIA33			
CAIA0219	BH	CAIA34			
CAIA2529	BI	CAIA35			
	BJ	CAIA36			
	BK	CAIA37			
	BL	CAIA38			
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	CR	CAIA70			
	CS	CAIA71			
	CT	CAIA72			
	CU	CAIA73			
	CV	CAIA74			
	AW	CAIA75			
	AX	CAIA76			
	AY	CAIA77			
	AZ	CAIA78			
	AA	CAIA79			
	AB	CAIA80			
	AC	CAIA81			
	AD	CAIA82			
	AE	CAIA83			
	AF	CAIA84			
	AG	CAIA85			
	AH	CAIA86			
	AI	CAIA87			
	AJ	CAIA88			
	AK	CAIA89			
	AL	CAIA90			
	AM	CAIA91			
	AN	CAIA92			
	AO	CAIA93			
	AP	CAIA94			
	AQ	CAIA95			
	AR	CAIA96			
	AS	CAIA97			
	AT	CAIA98			
	AU	CAIA99			
	AV	CAIA00			

Target Indicator: 8h Max daily O₃

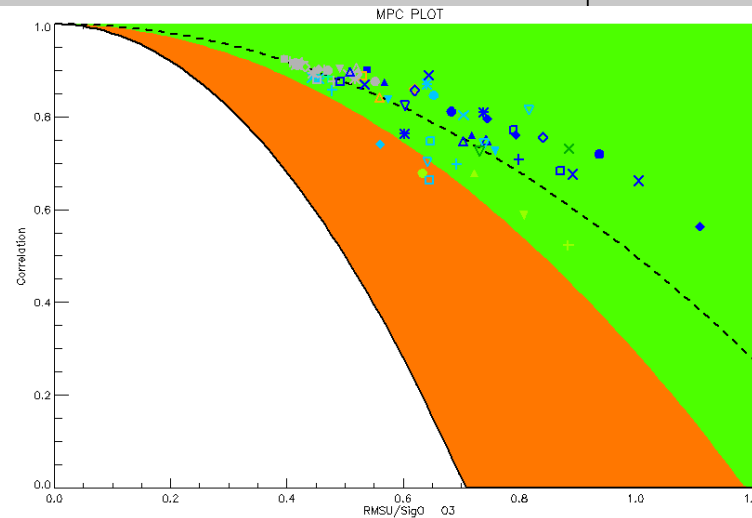
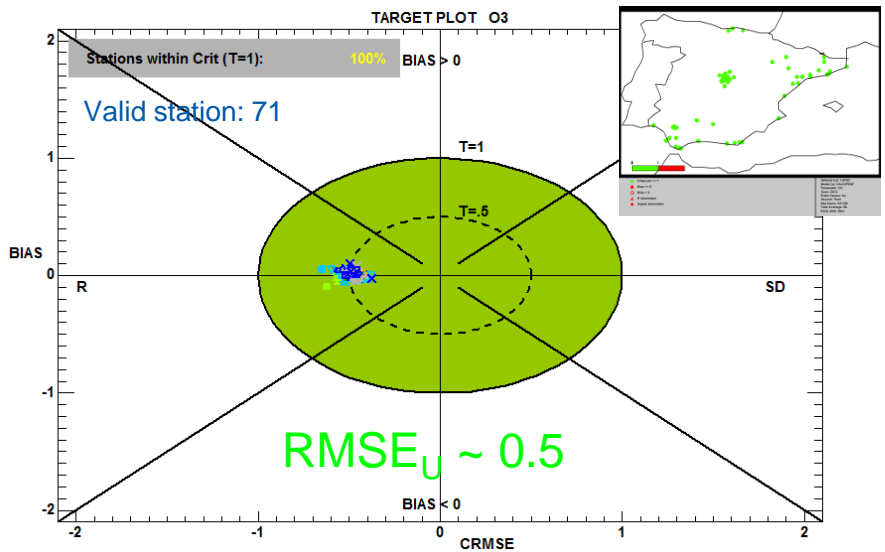
CALIOPE



A3	AY	CAIA2531	ES0010R	E51418A
AA	AZ	CAIA2533	E50118A	E51536A
AL	BC	CAIA2536	E50124A	E51537A
ALIA0011	BD	CAIA3200	E50126A	E51563A
ALIA0013	BJ	CAIA3600	E51182A	E51564A
ALIA0018	BK	CAIA3700	E51193A	E51565A
ALIA0021	BM	CAIA3900	E51386A	E51567A
AP	CO	COIA0006	E51400A	E51576A
AV	CAIA2510	COIA0007	E51417A	E51577A
	CAIA2529			

StrIend Id: 1-8760
Model (s): CALIOPE
Parameter: O₃
Scen: 2013
Extra Values: No
Season: Year
Day hours: All 24h
Time Average: 8h
Daily stats: Max

CALIOPEKF

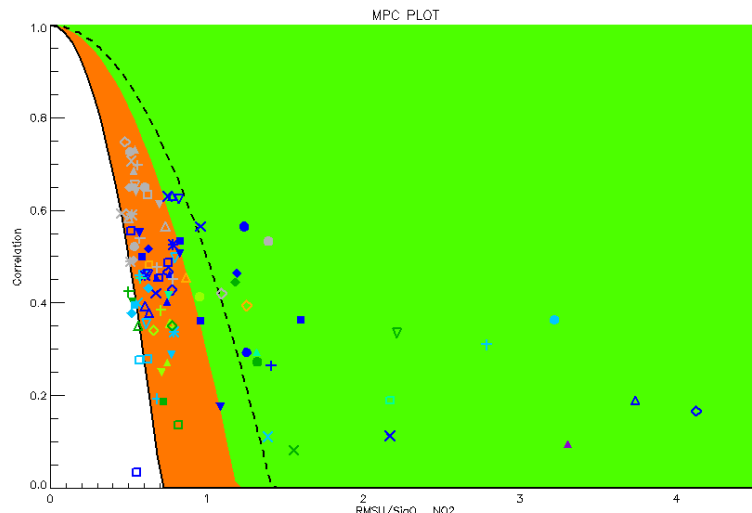
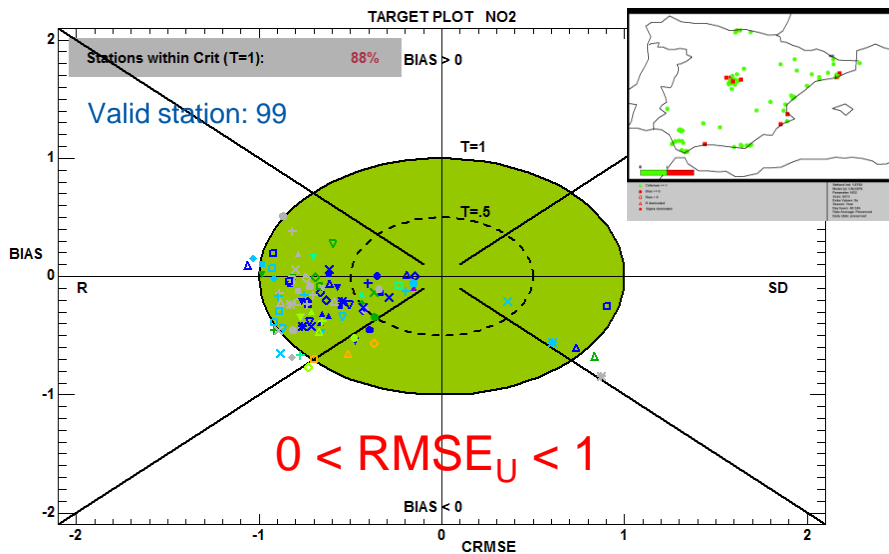


A3	AZ	CAIA2533	E50124A	E51565A
AA	BC	CAIA2536	E50126A	E51567A
AL	BD	CAIA3200	E51193A	E51576A
ALIA0011	BJ	CAIA3600	E51400A	E51577A
ALIA0013	BK	CAIA3700	E51417A	E51578A
ALIA0018	BM	CAIA3900	E51418A	E51579A
ALIA0021	CO	COIA0006	E51537A	E51611A
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AV	CAIA2529		E51564A	E51645A
AY	CAIA2531			

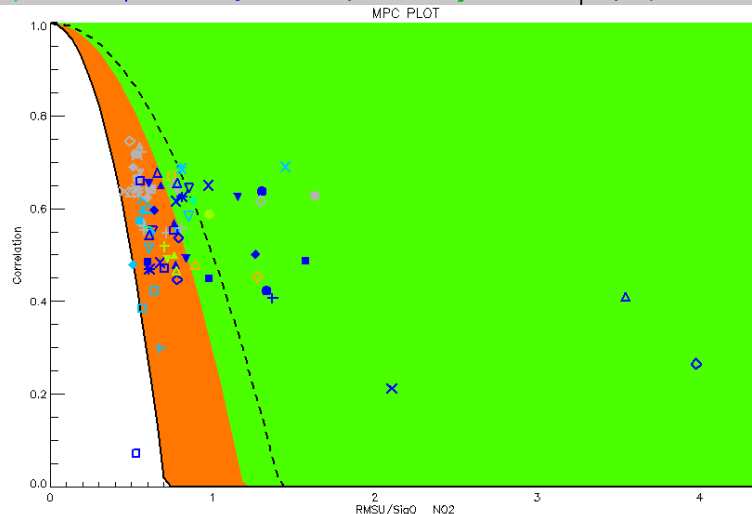
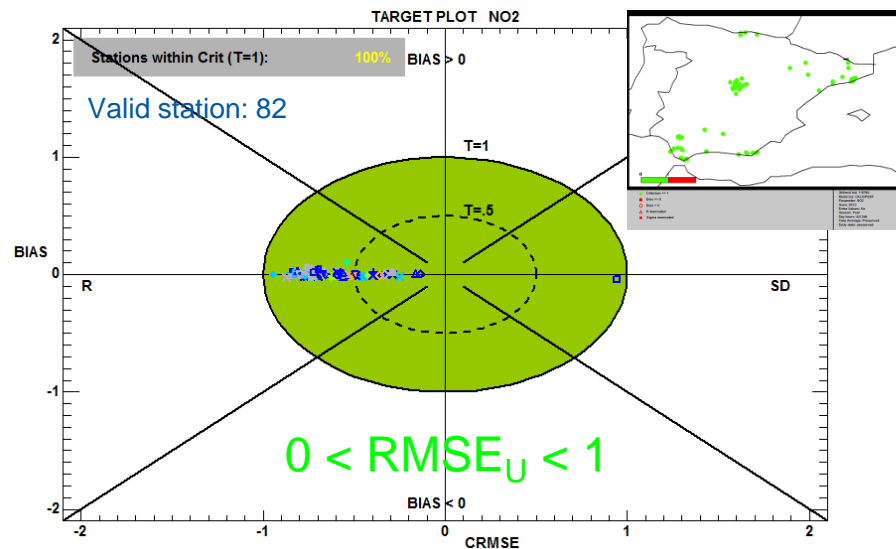
StrIend Id: 1-8760
Model (s): CALIOPEKF
Parameter: O₃
Scen: 2013
Extra Values: No
Season: Year
Day hours: All 24h
Time Average: 8h
Daily stats: Max

Target Indicator: hourly NO_2

CALIOPE



CALIOPEKF



Suggested MQO for forecast

Previously ...

$$\text{RMSE}_U = \frac{\sqrt{\frac{1}{N} \sum (O_i - M_i)^2}}{2U}$$

Evaluate if models are good enough based on observation uncertainty

New target indicator for forecast application (Thunis et al., 2012, FAIRMODE SG4 Report):

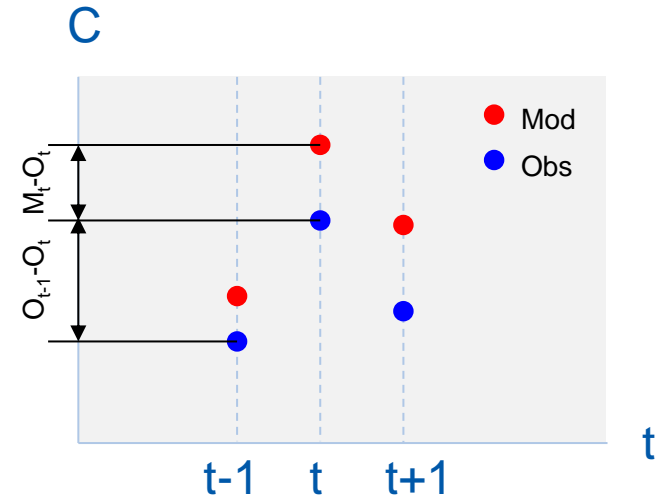
$$\text{Target} = \frac{\sqrt{\frac{1}{N} \sum_{i=1}^N (M_i - O_i)^2}}{\sqrt{\frac{1}{N} \sum_{i=1}^N (O_{i-1} - O_i)^2}}$$

Where N is the length of the time series.

“normalize by a quantity representative of the day-to-day variations”

- Comparison between $|M_t - O_t|$ vs $|O_{t-1} - O_t|$

Any sense?



- $O_{t-1} - O_t$ depends on:

- Δt = hourly, daily, annual, etc.
- Pollutant: e.g. O_3 marked daily cycle
- Station type: e.g. NO_2 daily cycle at UT vs remote rural background station
- Observation uncertainty of the pollutant: in forecast we work with no validated data!!

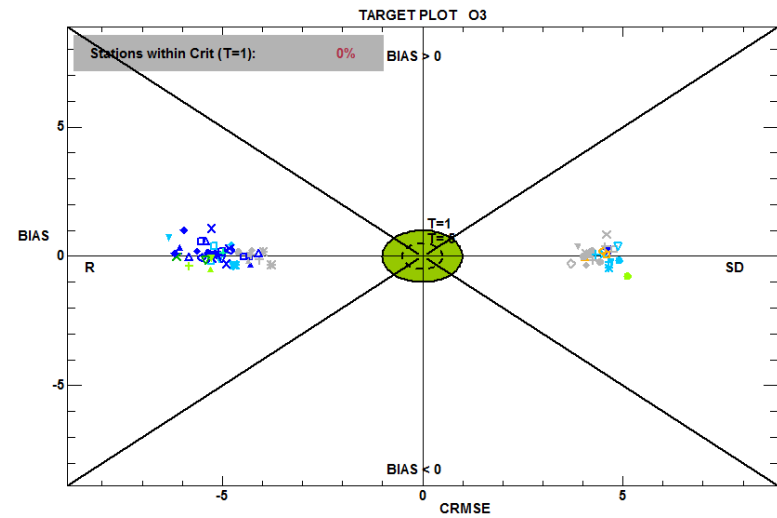
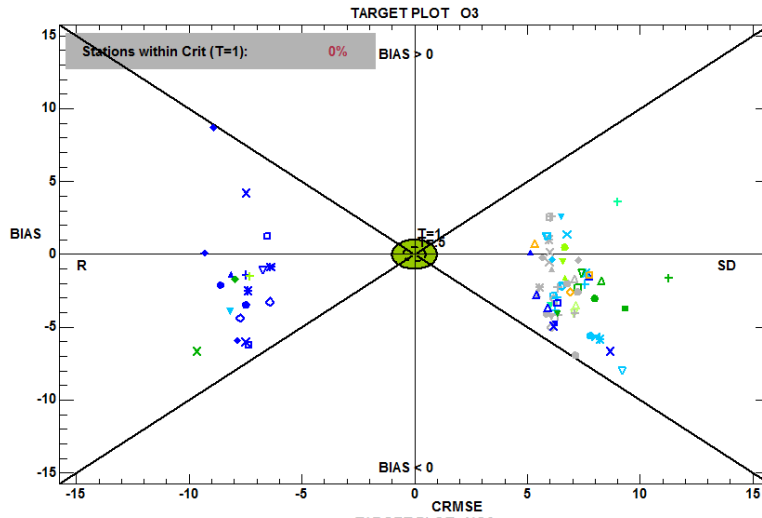
MQO for forecast in CALIOPE

$$\text{Target} = \sqrt{\frac{\frac{1}{N} \sum_{i=1}^N (M_i - o_i)^2}{\frac{1}{N} \sum_{i=1}^N (o_{i-1} - o_i)^2}}$$

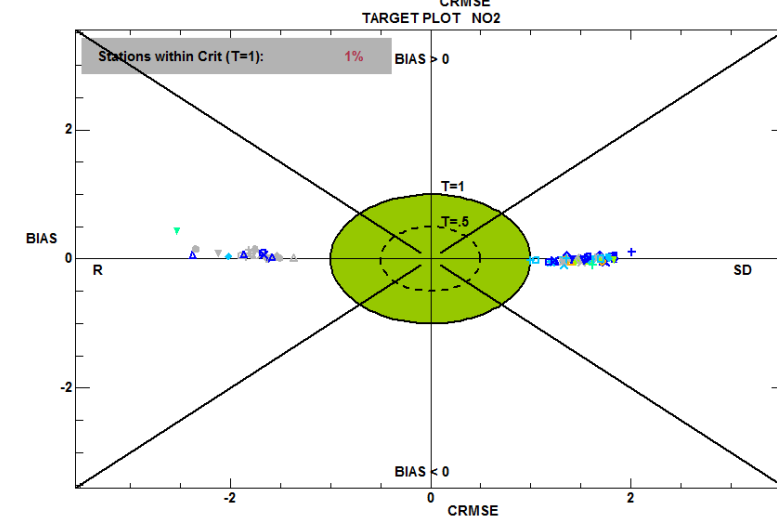
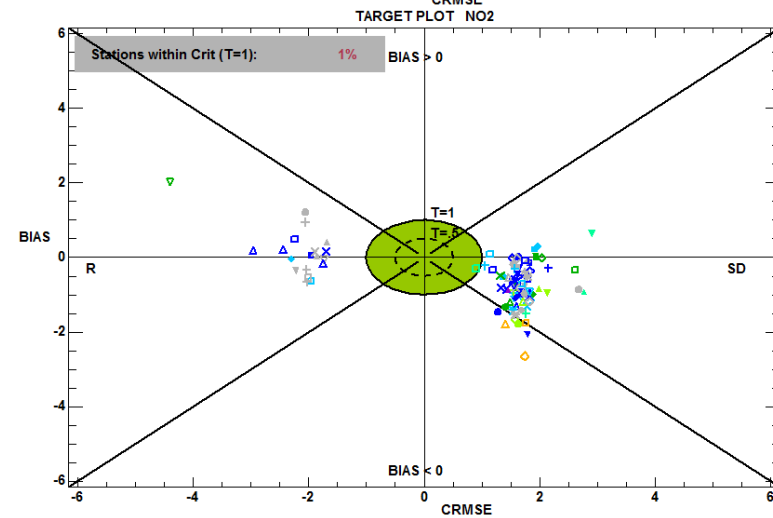
CALIOPE

CALIOPEKF

O₃ MAX 8h



NO₂ HOURLY



Conclusions and discussion (1/2)

❧ Evaluation of the effect of bias correction technique with Delta tool v 3.5. After applying KF (CALIOPE vs CALIOPEKF):

- Reduction of **annual mean bias** for O₃ (RB, ~10 ug/m³) and NO₂ (UT, ~7 ug/m³)
- Increasing of **annual r** from 0.5-0.6 to 0.8 in O₃ and 0.5-0.6 to 0.7-0.8 for NO₂.
- Higher agreement obs/mod for the **day/nigth variability**.
- **CALIOPE** fulfils the criterion for RMSE_U (< 1) for **8hMax O₃** (95%) but not for **Hourly NO₂** (only 88%)
- **CALIOPEKF** fulfils the criterion (100%) for **8hMax O₃** and **Hourly NO₂** to be acceptable for regulatory applications.

❧ New target for forecast applications:

- The normalization with the observation variability, does it significant sense?
- A new target for forecast (with regulatory orientation) should answer:
 - Is the model good enough to forecast exceedances of EU limit values?:
 - Categorical statistics (CSI, POD, FAR) suggested by Kang et al. (2005)
 - Categorical statistics normalized by area (aH, aFAR, WSI) suggested by Kang et al. (2007).
 - How the model performance degenerate with the forecast period (24h, 48h, 72h)? What is the confidence of that?

Conclusions and discussion (2/2)

About the DELTA tool v3.6

⌘ DELTA tool is useful for exploratory analysis:

- It harmonizes the evaluation techniques (e.g. statistic calculation) and it includes MQO acceptance.
- Representative statistical diagrams and indicators: e.g. Dynamic evaluation, spatial evaluation, GeoMap.

⌘ Suggestions:

- Problem with the preprocessor MODEL.csv to netcdf.csv_to_modeltypeV2.sav is working but with warnings.
- Indicate the number of stations (valid, selected, rejected) in each plot (e.g. in target plot).
- Valued outputs:
 - ~/DELTATOOL/dump/DumpFile.txt → Target plot
 - ~/DELTATOOL/dump/MODELNAME.txt → Summary Statistics
- Linux version? Scripting capabilities?

Thank you for your
attention

Contact: maria.pay@bsc.es