EVALUATION OF THE CHIMERE MODEL ESTIMATING WET DEPOSITION IN SPAIN

Fernando Martín, Marta G. Vivanco, Juan L. Garrido and Inmaculada Palomino

Atmospheric Pollution Division. CIEMAT,

Madrid, Spain

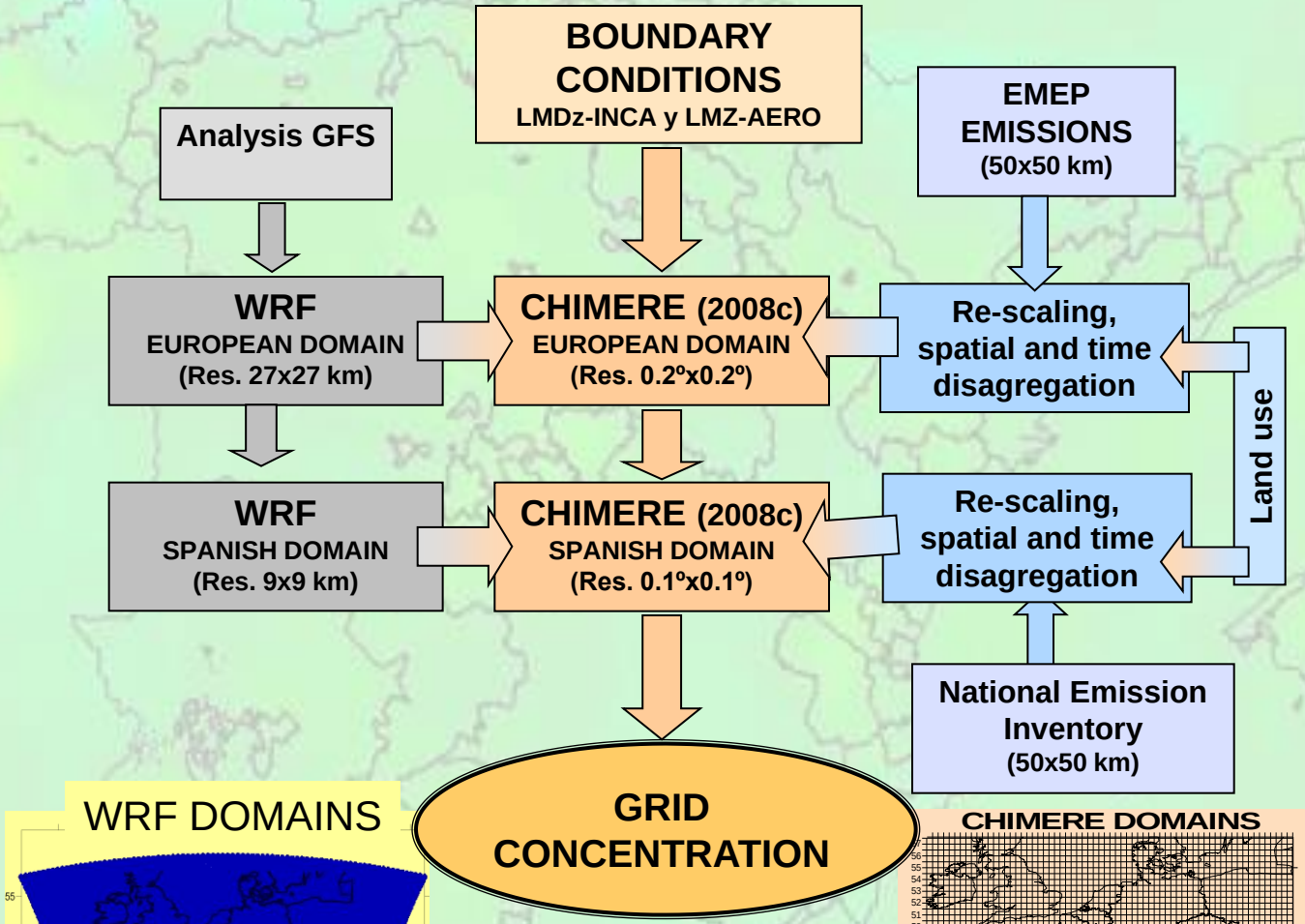
Introduction

- Few studies have been done to evaluate the ability of models to estimate pollutant deposition.
- Complex task because:
  - deposition is much more difficult to be accurately measured,
  - few stations.
- However, there are some studies about how models estimate the pollutant deposition (Simpson et al, 2006, Aas et al., 2010, Bessagnet et al, 2014 among others)

Objectives

- Evaluation of performance of CHIMERE estimating the wet deposition of sulphur and nitrogen (oxidized and reduced) on the Iberian Peninsula.
- Intercomparison with the EMEP model estimates.
- Main focus will be also on discussing seasonal and spatial variability.
- What is the main source of errors?

Methodology - Modeling scheme 2008



Methodology - Modeling

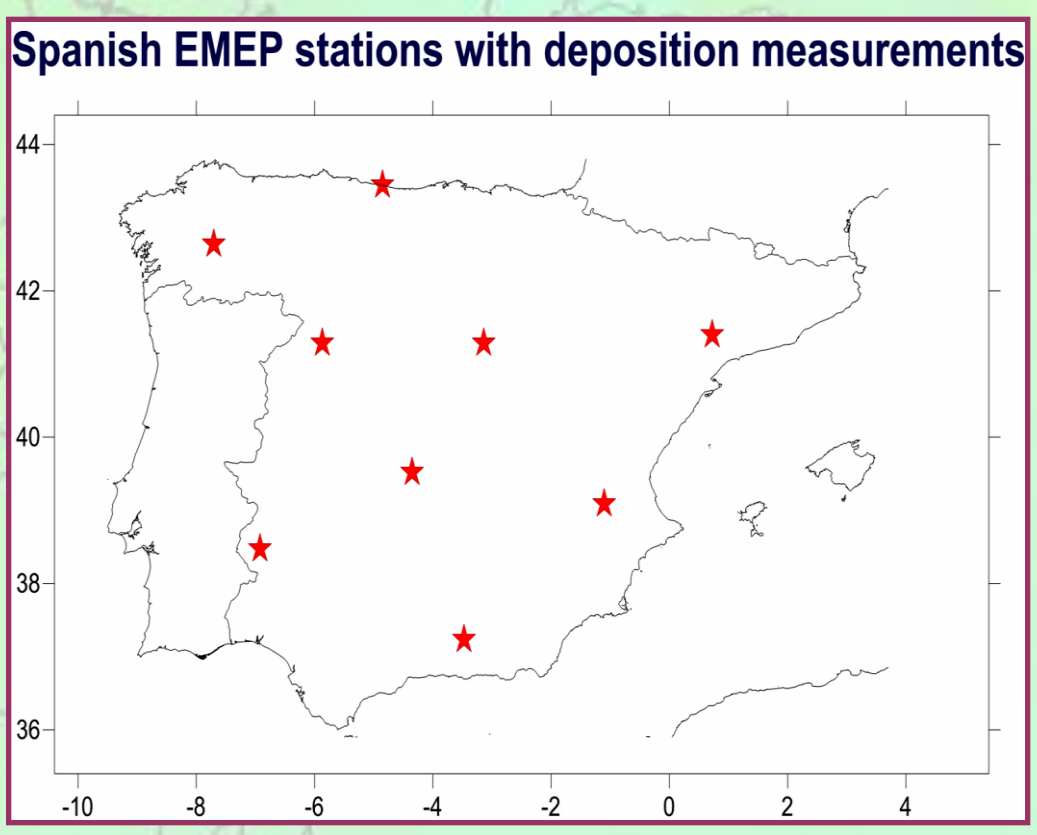
- CHIMERE simulations for 2005-2008. Spatial resolutions:
  - 2005-2007. European domain (0.5ºx0.5º grid resolution), Iberian Peninsula domain (0.2ºx0.2º resolution)
  - 2008. European domain (0.2ºx0.2º for 2008), Iberian Peninsula domain (0.1ºx0.1º km^2).
- Pollutant emission data from EMEP (50x50 km^2 resolution).
  - Disaggregated into hourly data in to the CHIMERE finer grid for the Iberian Peninsula using activity time profiles and land use data, respectively.
  - Spatial emission distribution and NMVOC speciation were performed as indicated in Vivanco et al. (2009).
- Wet deposition of sulfur and nitrogen (oxidized and reduced) on the Iberian Peninsula were estimated for the sites of the Spanish EMEP stations.

Methodology - Evaluation

- CHIMERE wet deposition estimates were compared with measured monthly data covering a period of 4 years (2005-2008).
- CHIMERE wet deposition estimates were also compared with EMEP estimates:
  - Annual atmospheric deposition data estimated for the period 2005–2008 with the EMEP model rv3.8.1 over Europe using a grid size of 50 km×50 km (Fagerli et al., 2011).
  - Meteorological data obtained from ECMWF-IFS Cycle36r1 (http://www.ecmwf.int/research/ifsdocs /)
  - Emissions from the EEA and CEIP Inventory Review of 2011.

Methodology – Evaluation – EMEP stations

- In Spain, the EMEP network 10 monitoring stations
- From sea level to 1360 m a.s.l.
- Daily samples of precipitation collected with wet-only samplers in 9 of the monitoring stations for the period 2005–2008.
- Measured deposition data accumulated throughout each month estimated following the EMEP protocols.



Methodology – Evaluation - Statistics

- Statistical metrics for time series of monthly data of wet deposition:
- Correlation coefficient (R),
- Mean fractional bias (MFB),
- Mean normalized factor bias (BNMBF) (Yu et al., 2006),

$$B_{NMBF} = \frac{\sum M_i}{\sum O_i} - 1 = \frac{\sum (M_i - O_i)}{\sum O_i} = \frac{\overline{M}}{\overline{O}} - 1 \text{ , if } \overline{M} \geq \overline{O} \text{ , and}$$

$$= (1 - \frac{\sum O_i}{\sum M_i}) = \frac{\sum (M_i - O_i)}{\sum M_i} = (1 - \frac{\overline{O}}{\overline{M}}) \text{, if } \overline{M} < \overline{O}$$

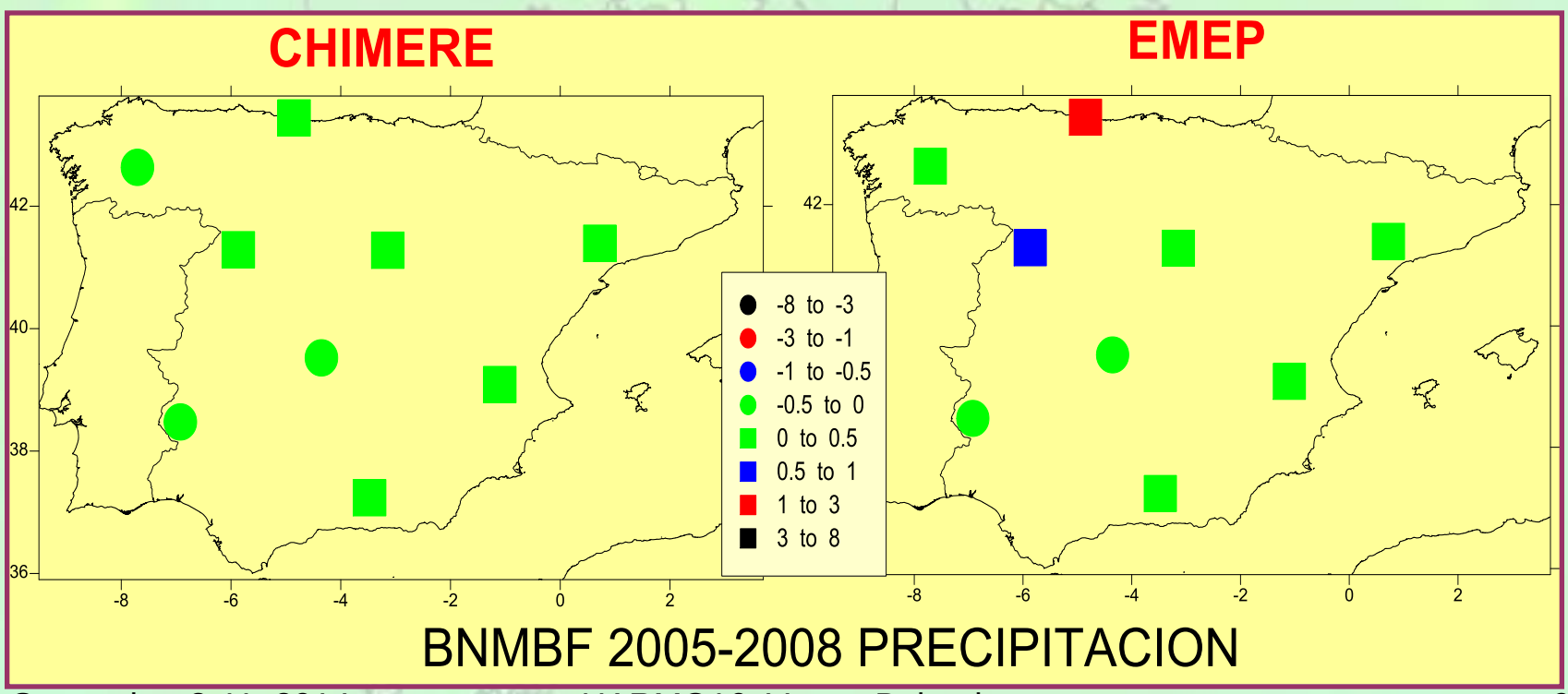
- **Variant of *MFB*, $-\infty \leq BNMBF \leq +\infty$**
- **Avoid impact of very low values of observations (O_i)**
- **Factor of overprediction = *BNMBF+1***
- **Factor of underprediction = 1-*BNMBF***

- Fraction of predictions within a factor of two of observations (FAC2),
- Normalized mean absolute error (NMAE)
- TARGET (Thunis et al., 2013) (RMSE/ standard deviation of observations)

Results – Monthly rainfall

- Meteorological models WRF and ECMWF-IFS linked to CHIMERE and EMEP, respectively.
- Both models predict well the monthly rainfall at most of the stations, specially the WRF model.

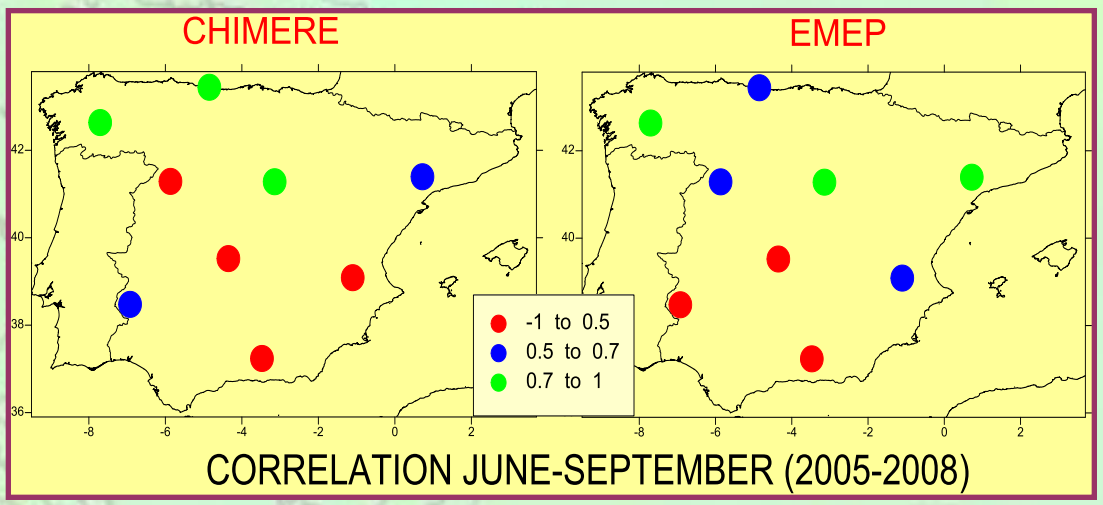
BNMBF values



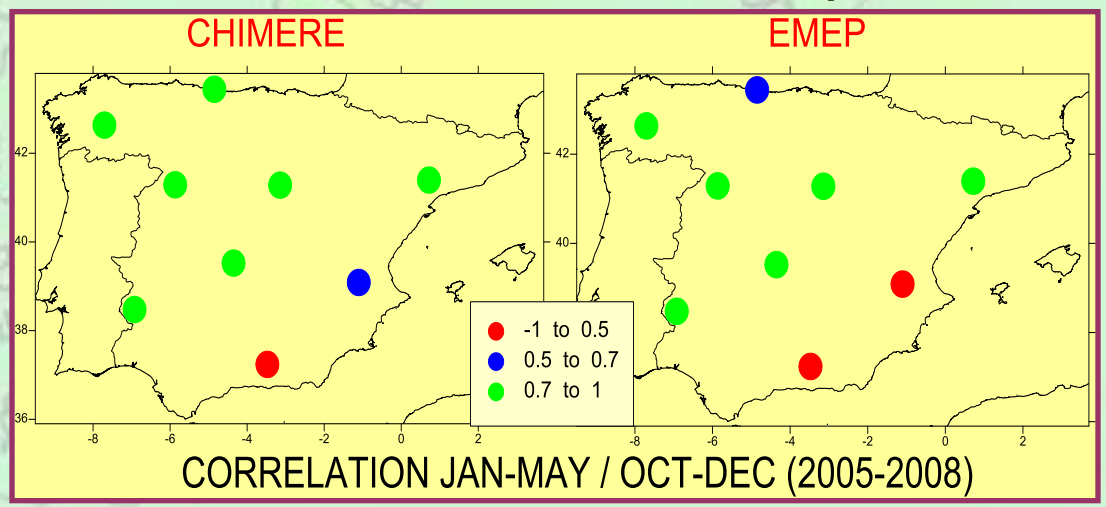
Results – Monthly rainfall

- Metrics slightly worse in summer time and at the South-Eastern stations:
  - most of precipitation is irregular small-scale convective (thunderstorms)
  - much more difficult to simulate
- Errors in predicting rainfall seem not to be the main cause of the errors found for sulfur and nitrogen deposition.

R values for the summer period (June-September)



R values for the non-summer period

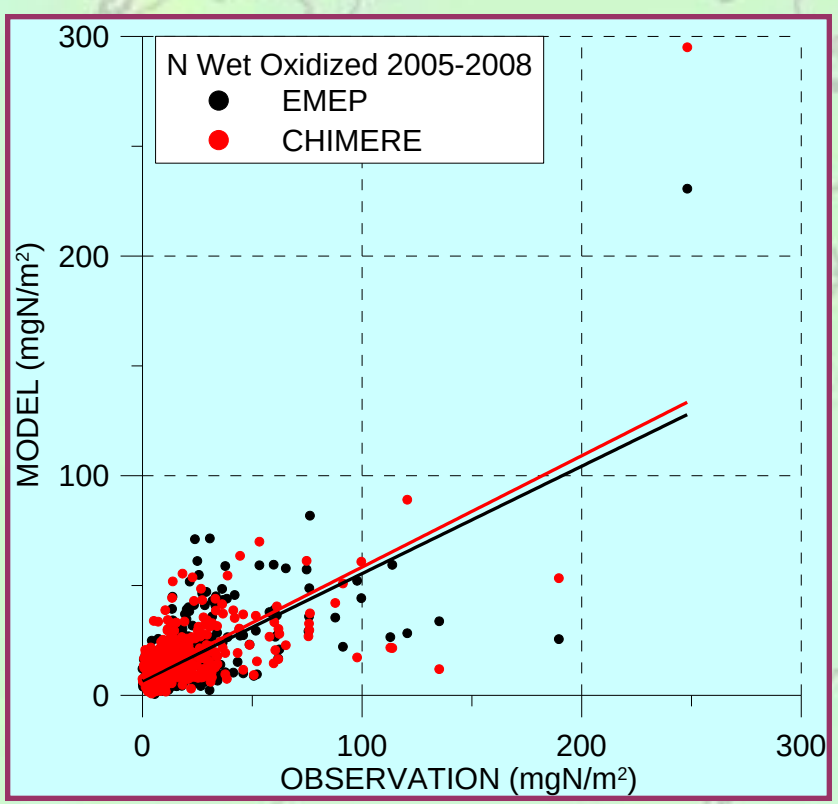


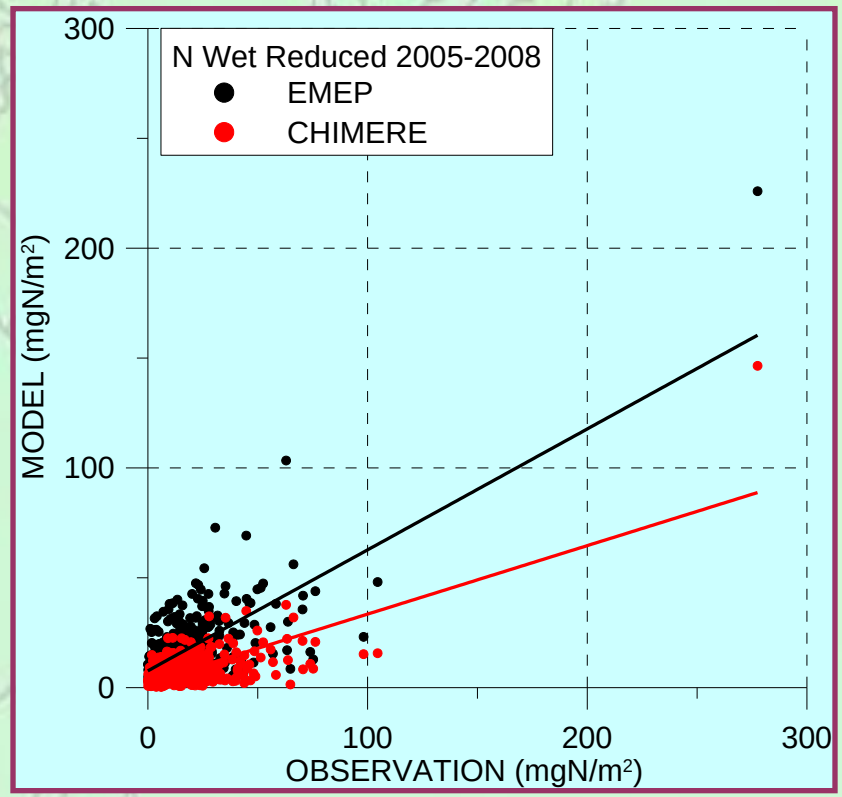
Results - Nitrogen - Statistics

- CHIMERE clearly underpredicts the wet deposition of reduced nitrogen (factor of 2.32) while the results for oxidized nitrogen are better than those of EMEP with a slight underprediction (factor of 1.14).

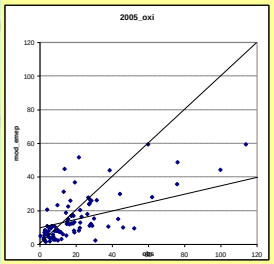
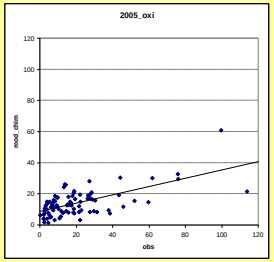
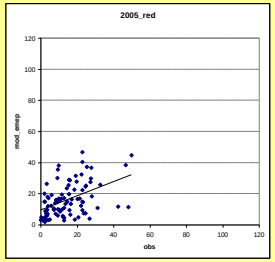
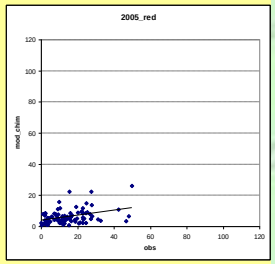
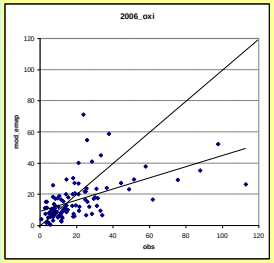
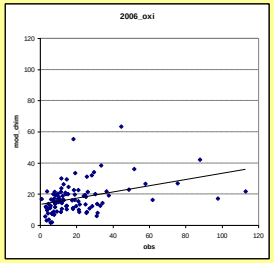
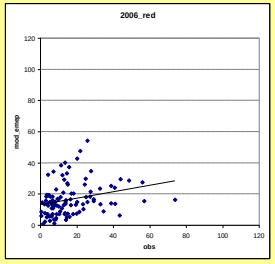
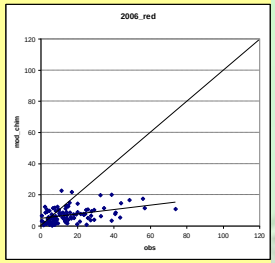
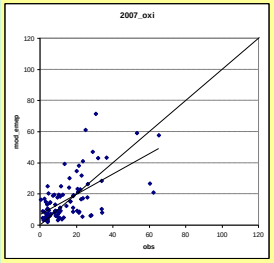
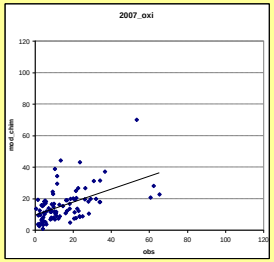
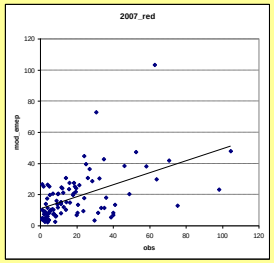
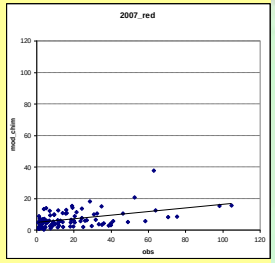
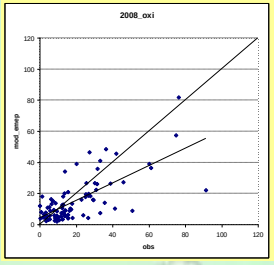
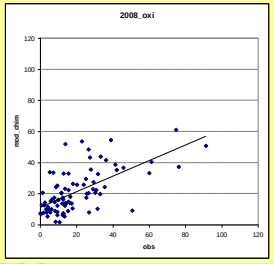
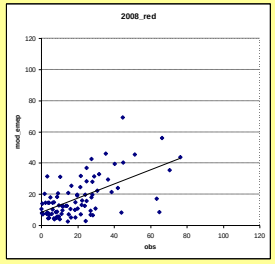
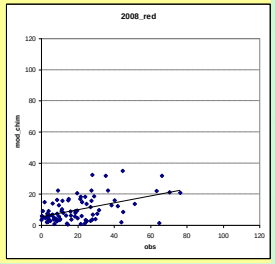
Metrics	CHIMERE REDUCED N	EMEP REDUCED N	CHIMERE OXIDIZED N	EMEP OXIDIZED N
R	0.44	0.48	0.54	0.56
MFB	-0.54	0.13	0.08	-0.1
BNMBF	-1.32	-0.02	-0.14	-0.24
FAC2	0.39	0.58	0.61	0.61
NMAE	0.67	0.6	0.56	0.53
Targets	1.09	0.92	0.85	0.85

Results - Nitrogen - Scatter Plots





Results - Nitrogen - Scatter Plots

	N OXIDIZED		N REDUCED	
	EMEP	CHIMERE	EMEP	CHIMERE
2005				
2006				
2007				
2008				

Results – Error contributions

- The amount of wet-deposited pollutant (*D*) is the result of several factors representing the rainfall (*P*), pollutant dispersion (including chemistry) and pollutant deposition (*DC*) processes:

$$D = P \cdot DC$$

- The relative error of deposition values ($\Delta D/D$) will be the summation of the relative errors of *P* and *DC*:

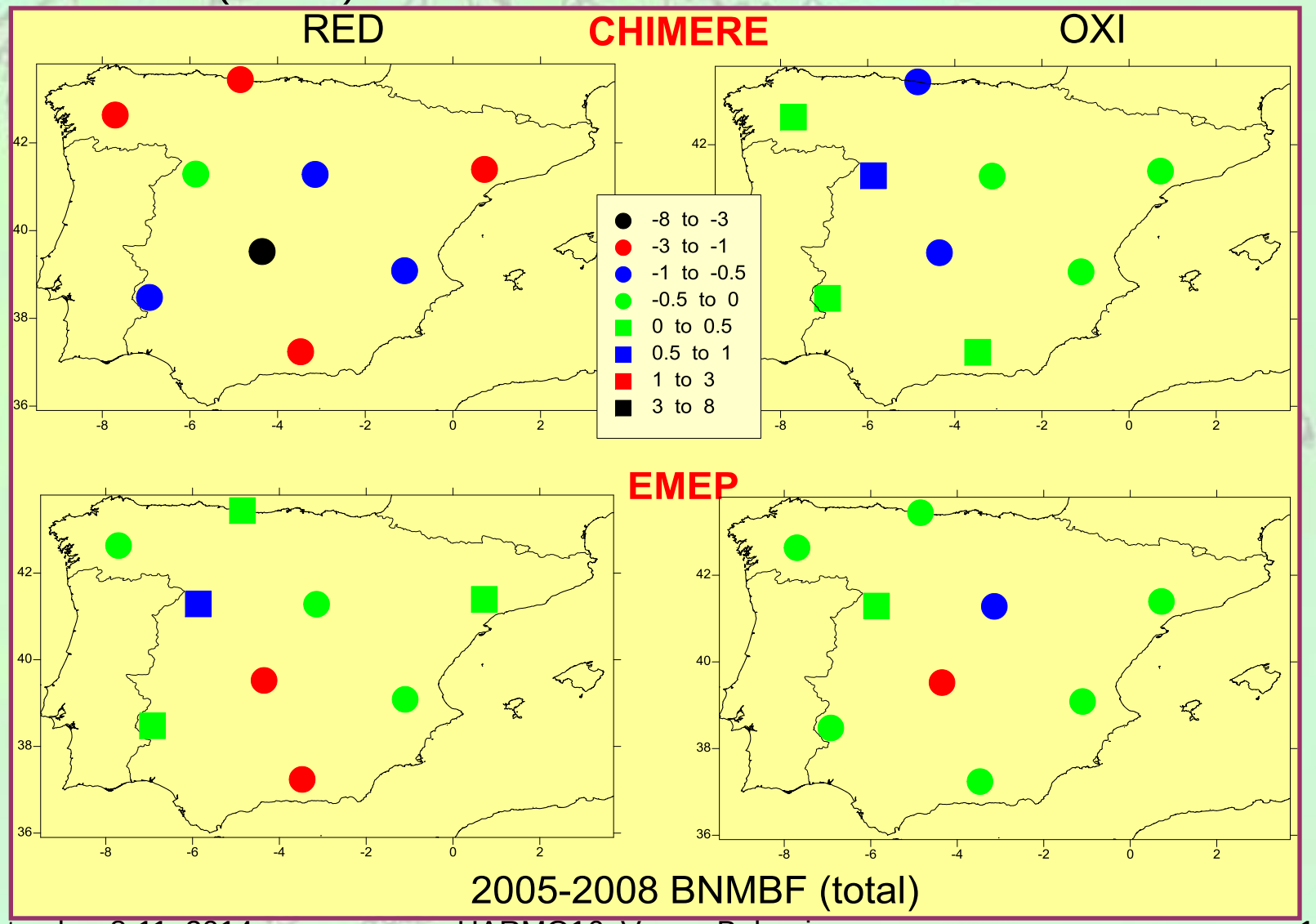
$$\frac{\Delta D}{D} = \frac{\Delta P}{P} + \frac{\Delta DC}{DC}$$

- Approximately, *BNMFBD = BNMFBP + BNMFBDC*
  - ***BNMFB*$_D$** = mean normalized factor bias of the deposition
  - ***BNMFB*$_P$** = mean normalized factor bias of the rainfall
  - ***BNMFB*$_{DC}$** = mean normalized factor bias of the dispersion (including chemistry)-deposition formulations,

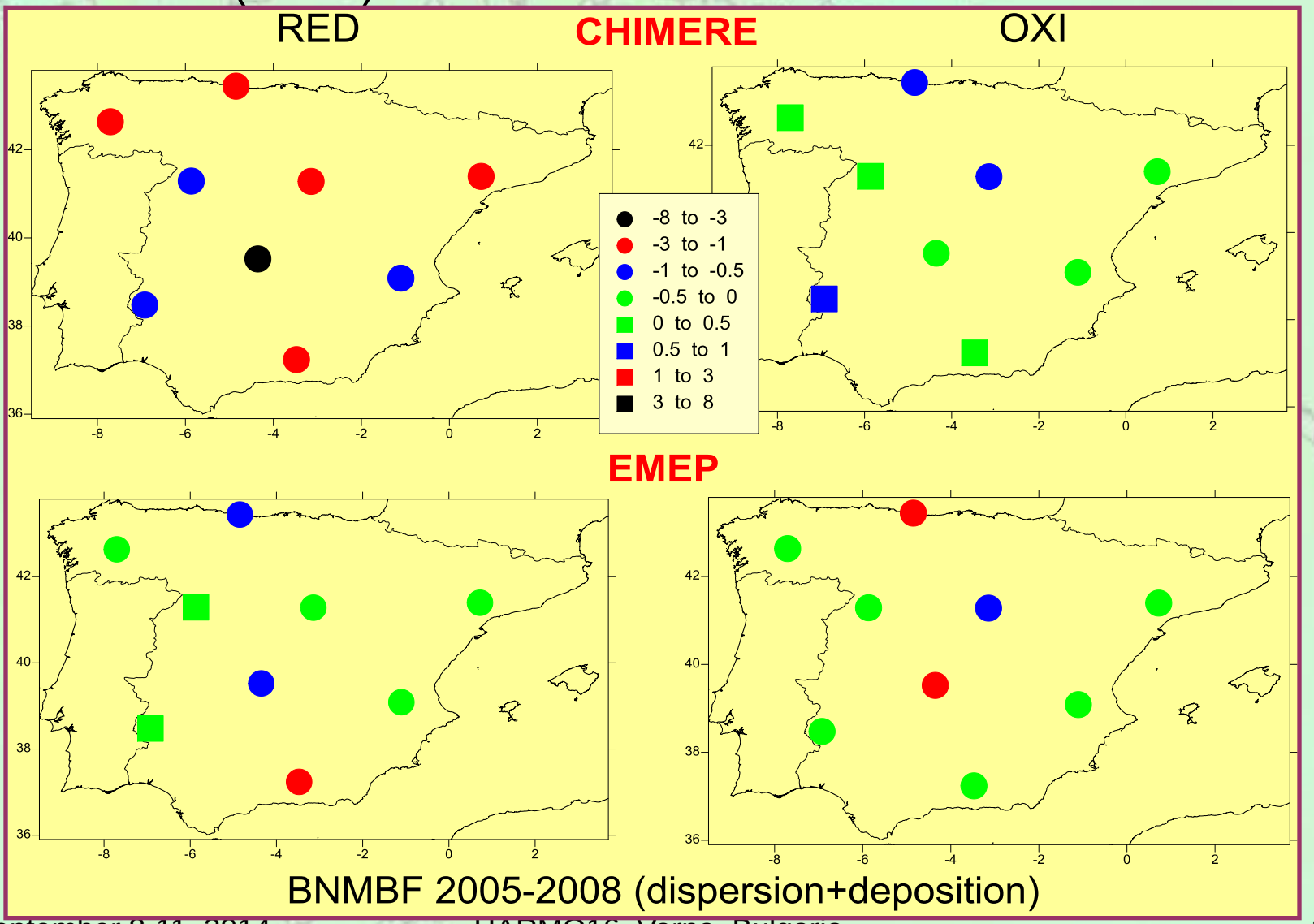
$$BNMFB_{DC} = BNMFB_D - BNMFB_P$$

- *BNMFB*$_D$ and *BNMFB*$_{DC}$ of the CHIMERE and EMEP estimates of wet deposition of oxidized and reduced nitrogen were computed for the 9 stations for 2005-2008.

$BNMFB_D$ of the wet deposition of reduced (left) and oxidized (right) nitrogen estimates obtained with the CHIMERE (above) and EMEP (below) at the EMEP stations for 2005-2008.



$BNMFB_{DC}$ of the wet deposition of reduced (left) and oxidized (right) nitrogen estimates obtained with the CHIMERE (above) and EMEP (below) at the EMEP stations for 2005-2008.

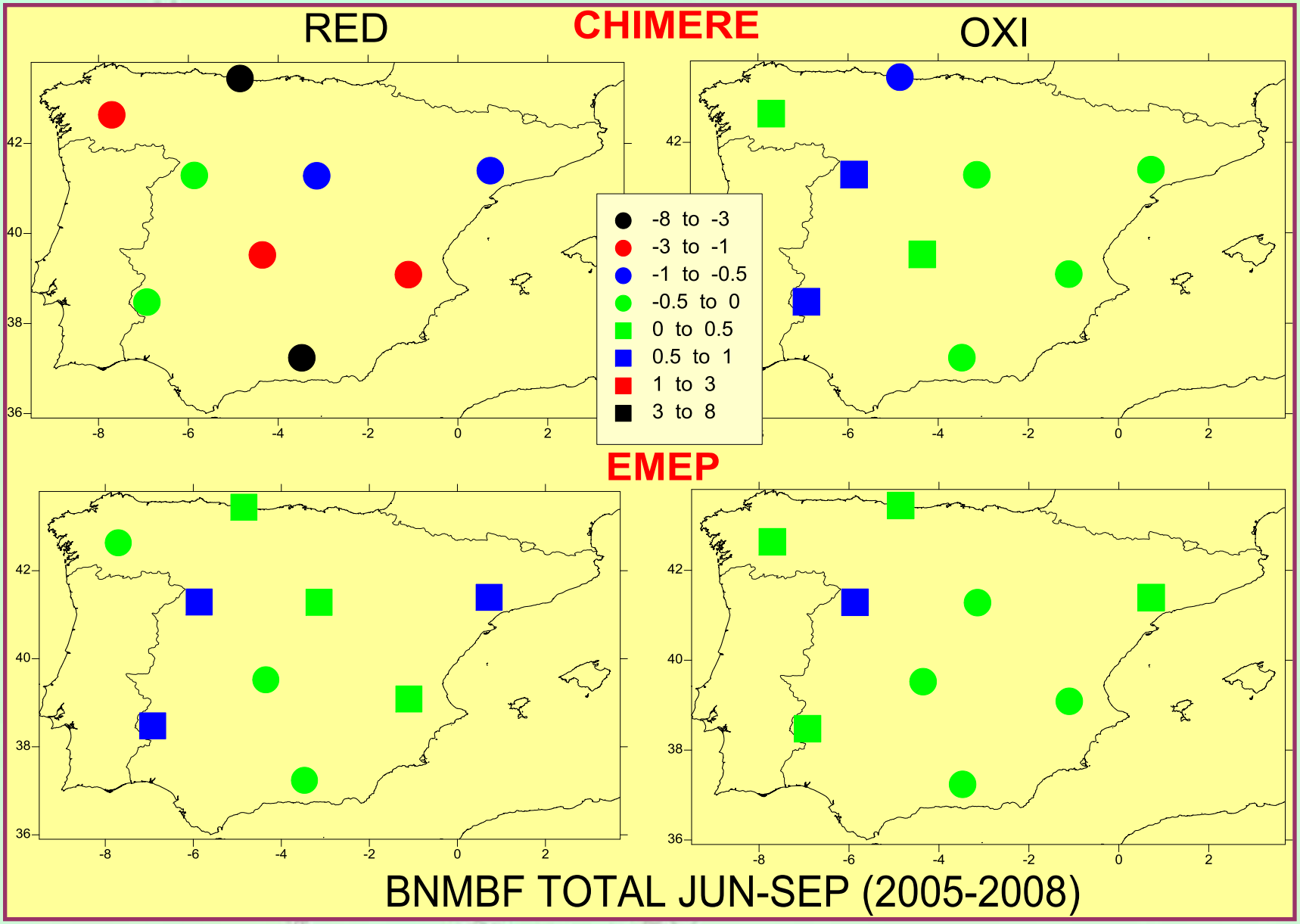


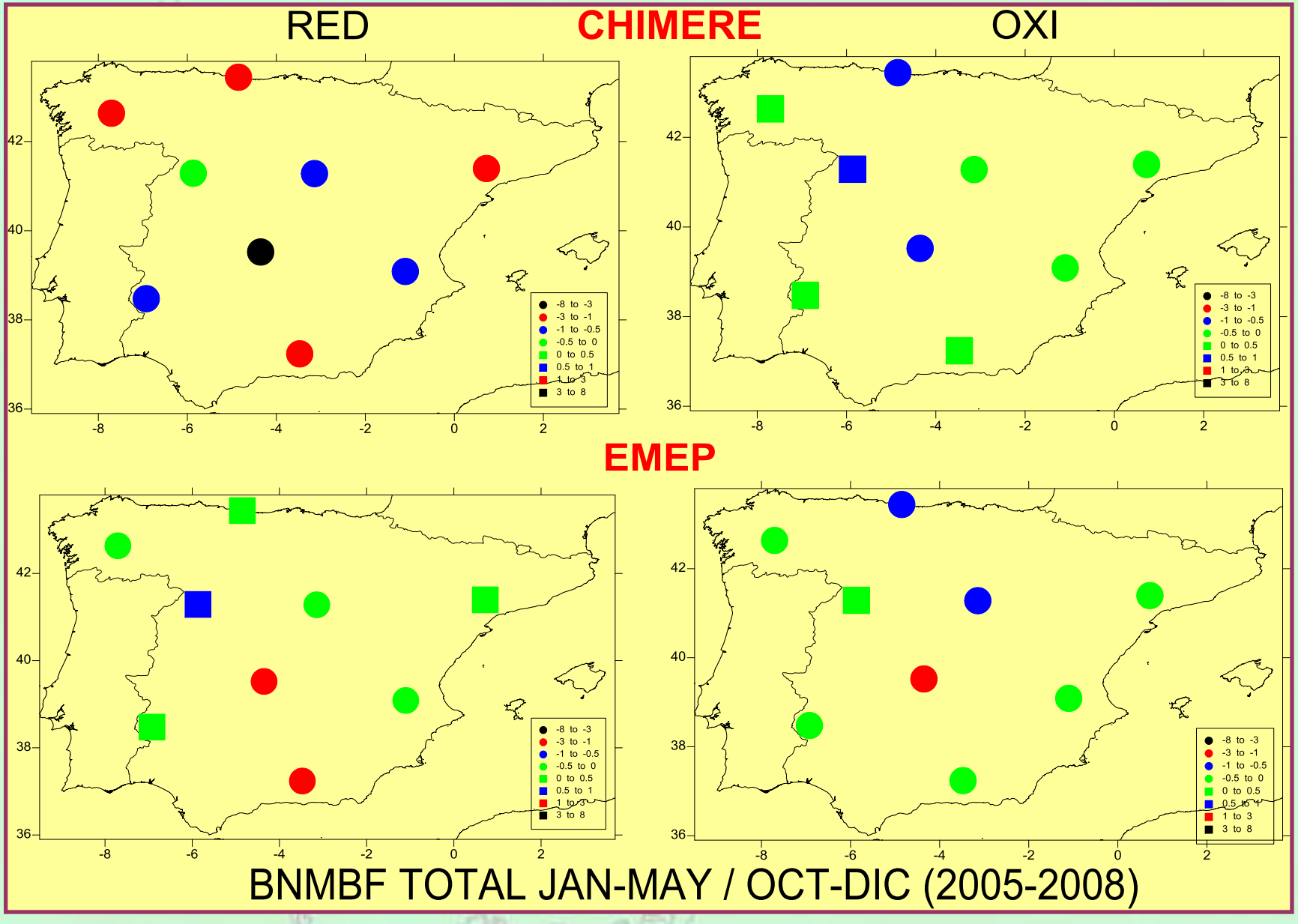
Results – Nitrogen – Error contributions

- Evident that underprediction of reduced nitrogen deposition estimated by CHIMERE is stronger when removing the effect of rainfall,
- Small changes are detected in the case of EMEP estimates.
- Concerning the oxidized nitrogen deposition, the highest impact is found for EMEP estimates, because the underprediction is extended to all the stations when removing the rainfall effect.
- It seems that the dispersion-chemistry-deposition formulations of EMEP model work slightly better for reduced nitrogen, and those of CHIMERE work better for oxidized nitrogen.

Results – Nitrogen – Seasonal

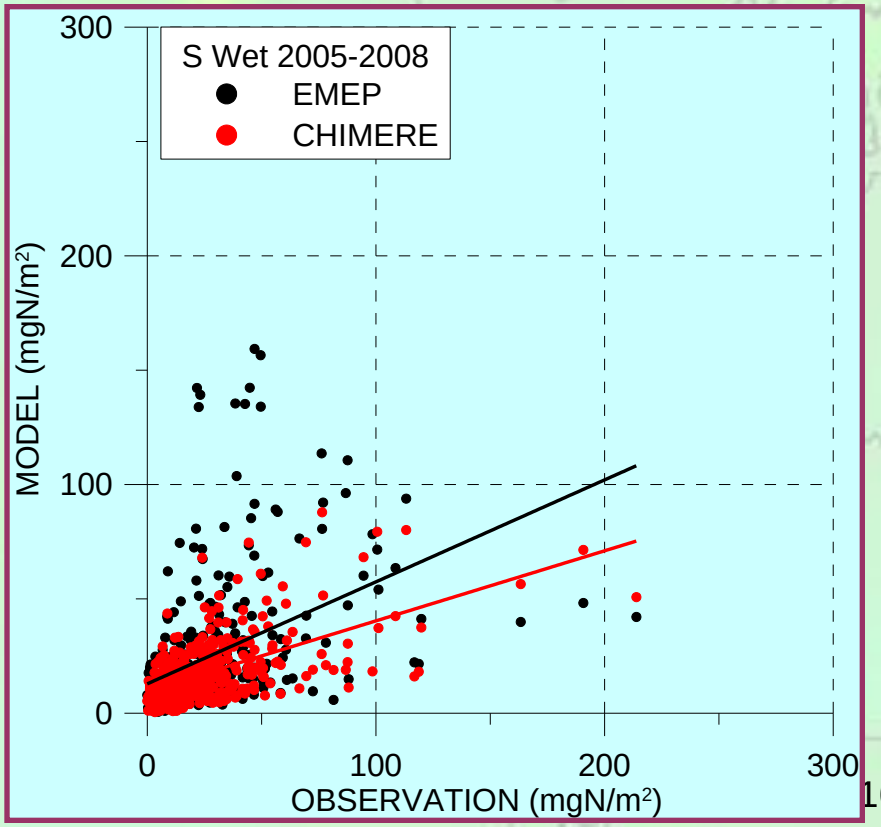
- Nitrogen wet deposition estimates with the EMEP model are better in summer
- Few differences in the case of the CHIMERE estimates of wet oxidized nitrogen deposition.
- There are some seasonal changes in the performance of CHIMERE for wet reduced nitrogen deposition for some stations but not in average in the whole domain.


RED
CHIMERE
OXI
EMEP
-8 to -3
-3 to -1
-1 to -0.5
-0.5 to 0
0 to 0.5
0.5 to 1
1 to 3
3 to 8
BNMBF TOTAL JUN-SEP (2005-2008)


RED
CHIMERE
OXI
EMEP
-8 to -3
-3 to -1
-1 to -0.5
-0.5 to 0
0 to 0.5
0.5 to 1
1 to 3
3 to 8
BNMBF TOTAL JAN-MAY / OCT-DIC (2005-2008)

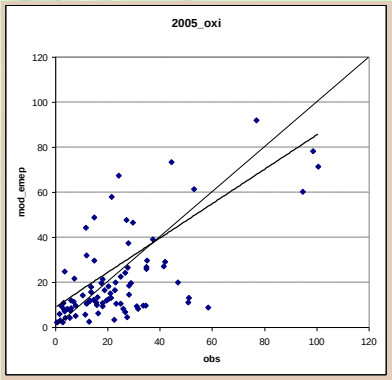
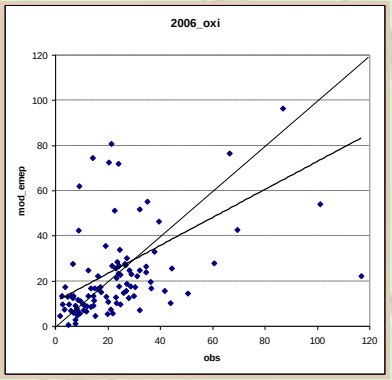
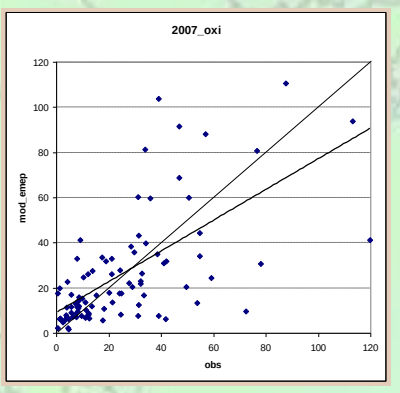
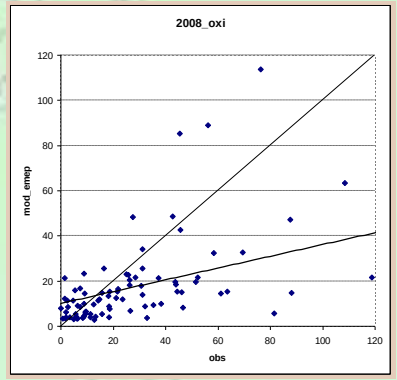
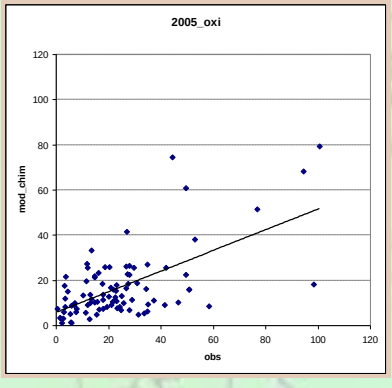
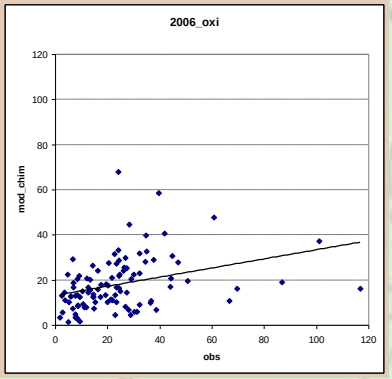
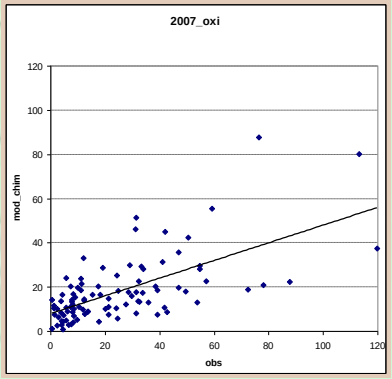
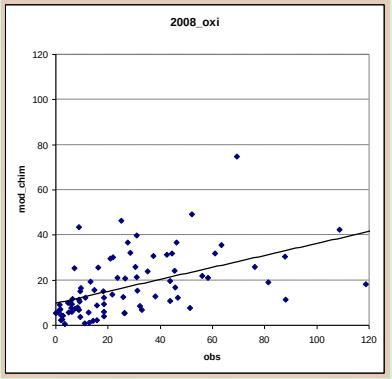
Results – Sulphur – Statistics – Scatter Plots

- CHIMERE estimates seem to correlate better with observations than those from EMEP.
- CHIMERE underpredicts more than EMEP, but metrics for errors are worse for EMEP.

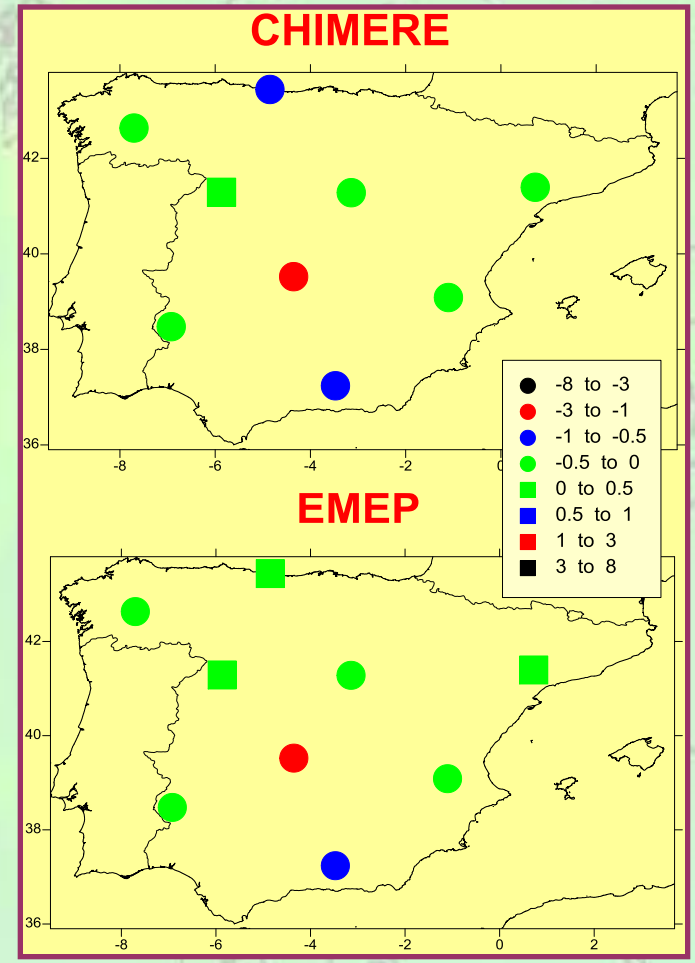


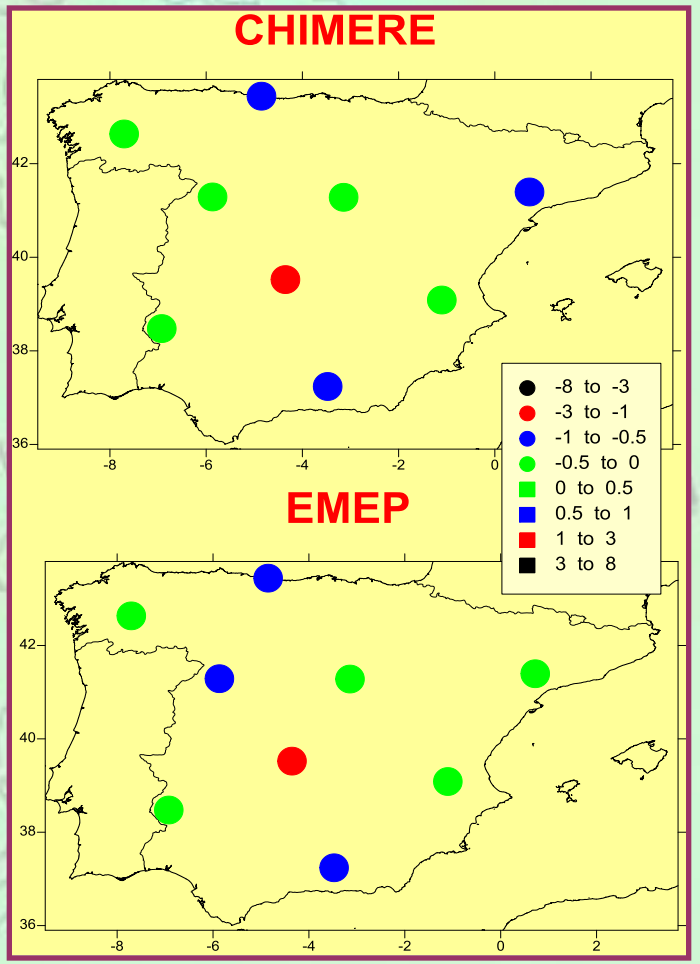
Metrics	CHIMERE Sulphur	EMEP Sulphur
R	0,55	0,43
MFB	-0,22	-0,06
BNMBF	-0,49	-0,07
FAC2	0,55	0,61
NMAE	0,56	0,63
Targets	0,89	1,09

Results – Sulphur – Scatter Plots

	2005	2006	2007	2008
EMEP				
CHIMERE				

BNMFB$_D$ (left) and *BNMFB*$_{DC}$ (right) of wet deposition of sulphur estimates obtained with the CHIMERE and EMEP for 2005-2008.





Errors in the estimation of rainfall were not the main cause of the estimation errors of wet sulfur deposition estimates.

Conclusions

- CHIMERE and EMEP provide quite acceptable wet deposition estimates of nitrogen (oxidized and reduced) and sulphur but there are things to improve.
- CHIMERE underpredicts the wet deposition of reduced nitrogen while the results for oxidized nitrogen are better than those of EMEP.
- Dispersion-chemistry-deposition formulations of EMEP model work better for reduced nitrogen, and those of CHIMERE work better for oxidized nitrogen.
- Some seasonal differences if the performance for nitrogen deposition, specially for EMEP model.
- For sulphur, CHIMERE has better correlation and error metrics than EMEP, but CHIMERE underpredicts more than EMEP.
- Meteorological models predict well the monthly rainfall, specially the WRF model. Worse results are for southeast and summer.
- Errors in predicting rainfall seem not to be the main cause of the errors found for sulfur and nitrogen deposition.

Thanks!