16th International Conference on
Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes
8-11 September 2014, Varna, Bulgaria

EVALUATION OF THE CHIMERE MODEL ESTIMATING WET DEPOSITION IN SPAIN

Martín F., Vivanco M.G., Garrido J.L Palomino I.

Atmospheric Pollution Division, CIEMAT, Avda. Complutense 40, 28040 Madrid, Spain

Abstract: The objective of this work is to do a comprehensive evaluation of how CHIMERE estimates the wet deposition of sulfur and nitrogen (oxidized and reduced) on the Iberian Peninsula. The CHIMERE estimates were compared with measured data in the Spanish EMEP stations on a monthly basis covering a period of 4 years (2005-2008). Statistical and graphical methods have been applied to analyze the model performance for the whole period and also the seasonal and spatial variability and compared with the results of the EMEP model. CHIMERE subpredicts the wet deposition of reduced nitrogen while the results for oxidized nitrogen are better than those of EMEP. CHIMERE estimates of wet deposition of sulfur seem to correlate quite well with observations in spite of there is slight subprediction. The rainfall estimates of meteorological models used by CHIMERE and EMEP fits quite well the observations with somewhat worse results in summer time and at Southeast stations. Errors in the estimation of precipitation seem not to be the main cause of the errors found for sulfur and nitrogen deposition.

Key words: *Model evaluation, pollutant deposition, sulfur, oxidized nitrogen, reduced nitrogen*.

INTRODUCTION

Few studies have been done for evaluating the ability of models to estimate pollutant deposition. This is a complex task because, unlike air pollutant concentrations: first, deposition is much more difficult to be accurately measured, and second, there are much fewer stations. However, there are some studies about how models estimates the pollutant deposition (Simpson et al, 2006, Aas et al., 2010, among others)

The objective of this work is to do a comprehensive evaluation of how CHIMERE estimates the wet deposition of sulfur and nitrogen (oxidized and reduced) on the Iberian Peninsula. The CHIMERE estimates were compared with measured data in the Spanish EMEP stations on a monthly basis covering a period of 4 years (2005-2008). Main focus will be also on discussing seasonal and spatial variability. A preliminary study, in which total annual N and S wet deposition estimates of the CHIMERE and EMEP models for Spanish stations were compared with measured data, can be seen in García et al (2014).

METHODOLOGY

CHIMERE was run for the 2005-2008 period over two nested domains: a European domain (50x50 km^2 grid resolution for 2005-2007 and 20x20 km^2 for 2008) and a finer domain focused on the Iberian Peninsula (20x20 km^2 resolution for 2005-2007 and 10x10 km^2 for 2008). WRF simulations were used as meteorological inputs. Boundary conditions were based onthe LMDZ-INCA and LMDZ-AERO models for CHIMERE and GFS model for WRF. Pollutant emission data were 50x50 km^2 resolution. This data were 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).

For this study, annual atmospheric nitrogen 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 were used (Fagerli et al., 2011). Meteorological data were obtained from ECMWF-IFS Cycle36r1 (http://www.ecmwf.int/research/ifsdocs/) and emissions from the EEA and CEIP Inventory Review of 2011.

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

Several statistical metrics such as correlation coefficient (R), mean fractional bias (MFB), mean normalized factor bias (BNMBF) (Yu et al., 2006), the fraction of predictions within a factor of two of observations (FAC2), normalized mean absolute error (NMAE) and TARGET (Thunis et al., 2013) were computed with the time series of wet deposition of oxidized and reduced nitrogen estimated by the models and measured at Spanish EMEP stations.

RESULTS AND DISCUSSION

As the estimated wet deposition strongly depends on simulated precipitation, the ability of the meteorological models (WRF and ECMWF-IFS, respectively) linked to CHIMERE and EMEP to estimate monthly rainfall was firstly analyzed. Both models predict well the monthly rainfall at most of the stations, specially the WRF model, but the results are slightly worse in summer time and at the South-Eastern stations (see figures 1 and 2). In both cases (in summer and in the Southeast), the irregular small-scale convective precipitation (thunderstorms) is frequent, becoming much more difficult its simulation. Errors in predicting rainfall seem not to be the main cause of the errors found for sulfur and nitrogen deposition.

Table 1 and Figure 3 show that CHIMERE clearly subpredicts 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).

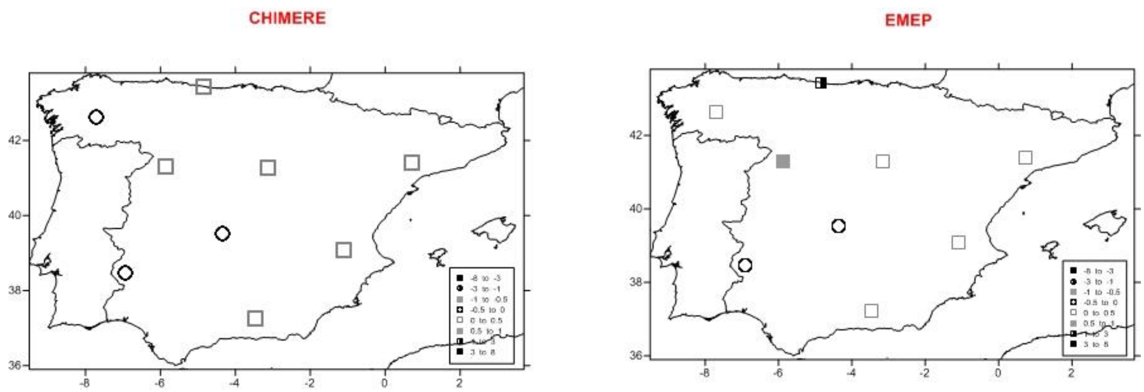

Figure 1. BNMBF values for the monthly rainfall estimated by the WRF (CHIMERE) and ECMWF/IFS (EMEP) models for 2005-2008.

Table 1. Values of the metrics from comparison of model and measured estimates of wet deposition of reduced and oxidized nitrogen and oxidized sulphur in Spain

Metrics	CHIMERE REDUCED N	EMEP REDUCED N	CHIMERE OXIDIZED N	EMEP OXIDIZED N	CHIMERE OXIDIZED S	EMEP OXIDIZED S
R	0.44	0.48	0.54	0.56	0,55	0,43
MFB	-0.54	0.13	0.08	-0.1	-0,22	-0,06
BNMBF	-1.32	-0.02	-0.14	-0.24	-0,49	-0,07
FAC2	0.39	0.58	0.61	0.61	0,55	0,61
NMAE	0.67	0.6	0.56	0.53	0,56	0,63
Targets	1.09	0.92	0.85	0.85	0,89	1,09

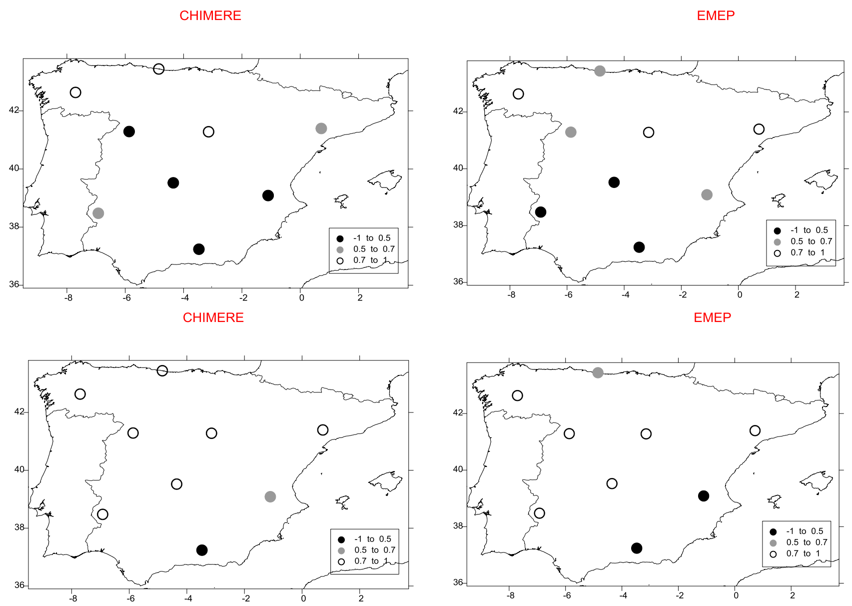

Figure 2. R values for the monthly rainfall estimated by the WRF (CHIMERE) and ECMWF/IFS (EMEP) models for the summer period (June-September) (above) and non-summer period for 2005-2008.

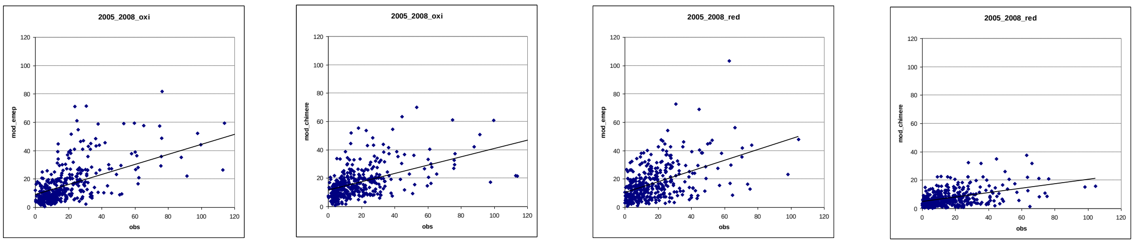

Figure 3. Scatter plots (observation vs modelled data) of monthly wet deposition of reduced nitrogen for the CHIMERE model (left) and EMEP model (centre left) and of oxidized nitrogen for the CHIMERE model (centre right) and EMEP model (right) for 2005-2008.

The amount of wet-deposited pollutant (D) is the result of several factors representing the rainfall, pollutant dispersion (including chemistry) and pollutant deposition processes. Then, let say that:

$$D = P \cdot DC$$

where P represents the rainfall process and DC is the combination of dispersion and deposition process in model formulations. The relative error of deposition values ($\Delta D/D$) will be the summation of the relative errors of P and DC:

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

Metrics related to normalized bias are very similar to relative errors. Hence, approximately, we can say that:

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

being $BNMFB_D$, $BNMFB_P$ and $BNMFB_{DC}$ the mean normalized factor bias of the deposition values, rainfall values and those related to dispersion(including chemistry)-deposition formulations, respectively. $BNMFB_D$ and $BNMFB_P$ are computed directly by comparing measured and modelled data of deposition and rainfall. Hence, $BNMFB_{DC}$ can be estimated by subtracting $BNMFB_D$ - $BNMFB_P$.

In figures 4 and 5, the values of $BNMFB_D$ and $BNMFB_{DC}$ of the CHIMERE and EMEP estimates are shown for the 9 stations and for 2005-2008. It seems evident that subprediction of reduced nitrogen deposition estimated by CHIMERE is stronger when removing the effect of rainfall, while 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 subprediction is extended to all the stations when removing the rainfall effect. It seems that the dispersion-chemistry-deposition formulations of EMEP model work better for reduced nitrogen, and those of CHIMERE work better for oxidized nitrogen. It was noted that nitrogen wet deposition estimates with the EMEP model are better in summer, but there are not differences in the case of the CHIMERE estimates.

Concerning the wet deposition of sulphur, CHIMERE estimates seem to correlate better with observations than those from EMEP. CHIMERE subpredicts more than EMEP, but metrics for errors are worse for EMEP (see table 1 and figure 6). As for the case of nitrogen deposition, it has been shown that the errors in the estimation of rainfall were not the main causes of the estimation errors of sulfur deposition estimates.

More research is necessary to achieve a better estimation of pollutant deposition. This seems pretty clear in the case of CHIMERE model to estimate wet deposition of reduced nitrogen. However, we must also take into account the uncertainty of the deposition measurement methods, superior to the measurement of air pollutant concentration, which is an additional difficulty to the adequate assessment of models.

ACKNOWLEDGEMENTS

This study was also supported by the Spanish Ministry of Agriculture, Food and Environment. The authors thank Hilde Fagerli, Svetlana Sciro and Anna Benedictow for their helpful comments and suggestions.

REFERENCES

Aas W, Solberg S, Gauss M, Simpson D., 2010: The Mediterranean Region. Transboundary acidification, eutrophication and ground level ozone in Europe in 2008. EMEP status report 1/2010 Oslo, Norway: The Norwegian Meteorological Institute; p. 99–104.

Fagerli H, Gauss M, Benedictow A, Griesfeller J, Jonson JE, Nyiri A, et al., 2011: Transboundary acidification, eutrophication and ground level ozone in Europe in 2009. EMEP Status. Report 1/2011. Oslo: Norwegian Meteorological Institute; 127 pp..

García-Gómez H., J.L. Garrido , M.G. Vivanco, L. Lassaletta, I. Rábago, A. Àvila, S. Tsyro, G. Sánchez , A. González Ortiz, I. González-Fernández, R. Alonso, 2013: Nitrogen deposition in Spain: Modeled patterns and threatened habitats within the Natura 2000 network. *Science of the Total Environment* **485–486**, 450–460

Simpson D, Fagerli H, Hellsten S, Knulst JC, Westling O. Comparison of modelled and monitored deposition fluxes of sulphur and nitrogen to ICP-forest sites in Europe. *Biogeosciences*; **3**: 337–55.

Thunis P., A. Pederzoli, E. Georgievia, C. Cuvelier, D. Pernigotti, 2012: DELTA V3.0 User Guide. Joint Research Centre, Ispra, 55p

Vivanco MG, Palomino I, Vautard R, Bessagnet B, Martín F, Menut L, Jiménez S (2009) Multi-year assessment of photochemical air quality simulation over Spain. *Environmental Modelling & Software* **24**: 63-73

Yu S., Eder B., Dennis R., Chu S.H. and Schwartz S.E., 2006, New unbiased symmetric metrics for evaluation of air quality models. *Atmos. Sci. Let*. **7**: 26–34.

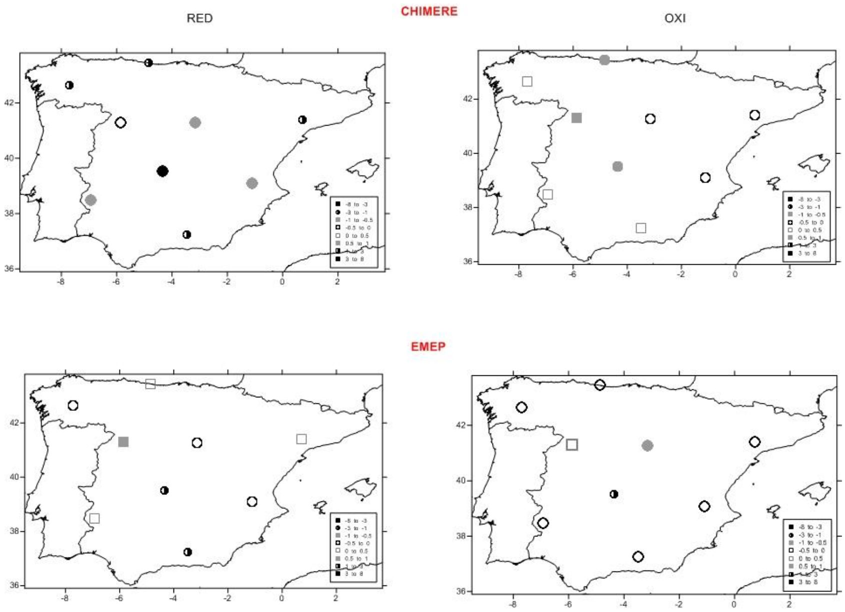

Figure 4. $BNMFB_D$ of the wet deposition of reduced (left) and oxidized (right) nitrogen estimates obtained with the CHIMERE (above) and EMEP (below) at the EMEP stations for 2005-2008.

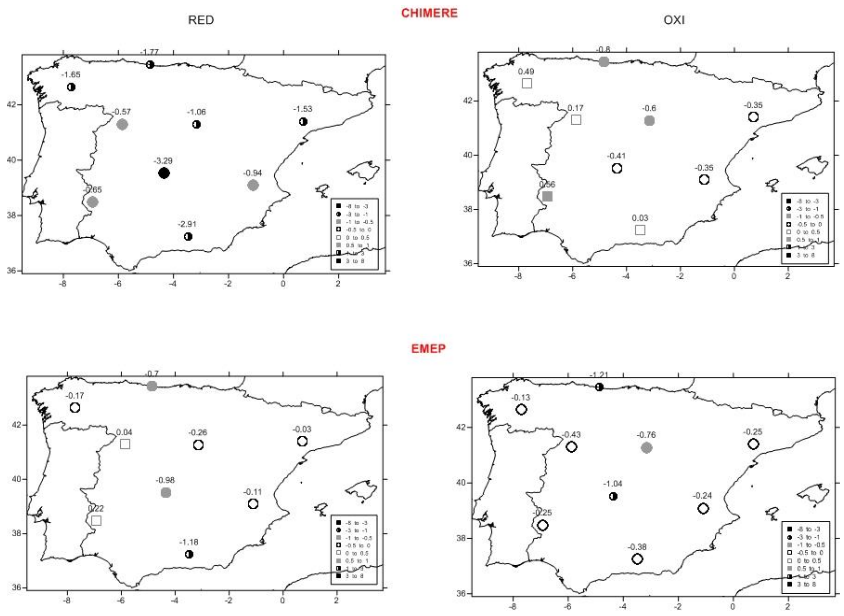

Figure 5. $BNMFB_{DC}$ of the wet deposition of reduced (left) and oxidized (right) nitrogen estimates obtained with the CHIMERE (above) and EMEP (below) at the EMEP stations for 2005-2008.

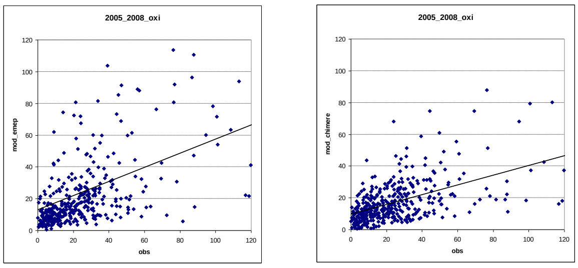

Figure 6. Scatter plots (observation vs modelled data) of monthly wet deposition of oxidized sulphur for the CHIMERE model (left) and EMEP model (right) for 2005-2008.

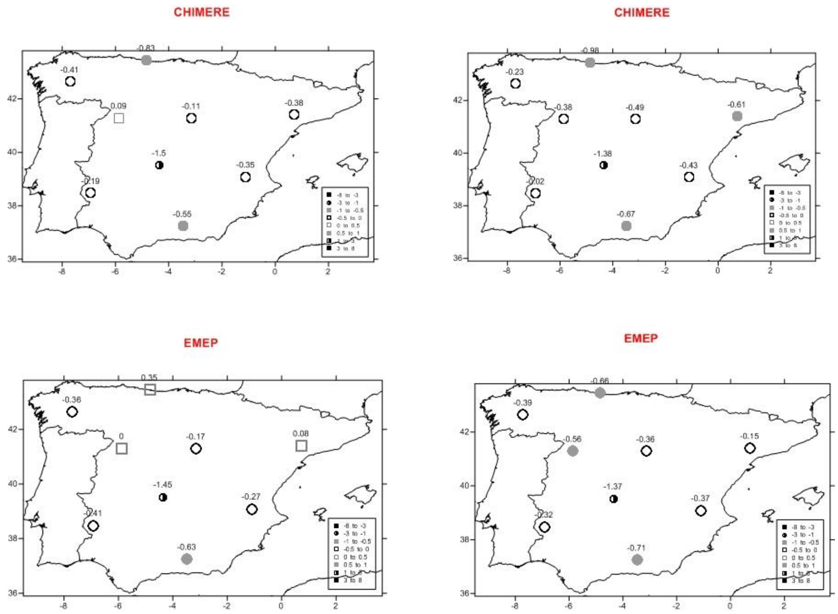

Figure 7. $BNMFB_D$ (left) and $BNMFB_{DC}$ (right) of the wet deposition of oxidized sulphur with the CHIMERE (above) and EMEP (below) at the EMEP stations for 2005-2008.