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

- **Boundary Conditions**: LMDz-INCA y LMZ-AERO
- **Chimere (2008c)**
  - European Domain: Res. 0.2°x0.2°
  - Spanish Domain: Res. 0.1°x0.1°
- **WRF Domains**
  - European Domain: Res. 27x27 km
  - Spanish Domain: Res. 9x9 km
- **Grid Concentration**
- **WRF**
- **Chimere Domains**
- **EMEP Emissions**: (50x50 km)
- **Re-scaling, spatial and time disaggregation**
- **Land use**
- **National Emission Inventory**: (50x50 km)
- **Analysis GFS**
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 km²).

• Pollutant emission data from EMEP (50x50 km² 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),

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

\[ = (1 - \frac{\sum O_i}{\sum M_i}) = \frac{\sum (M_i - O_i)}{\sum M_i} = (1 - \frac{\bar{O}}{M}), \text{ if } M < \bar{O} \]

- 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.
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).

<table>
<thead>
<tr>
<th>Metrics</th>
<th>CHIMERE REDUCED N</th>
<th>EMEP REDUCED N</th>
<th>CHIMERE OXIDIZED N</th>
<th>EMEP OXIDIZED N</th>
</tr>
</thead>
<tbody>
<tr>
<td>R</td>
<td>0.44</td>
<td>0.48</td>
<td>0.54</td>
<td>0.56</td>
</tr>
<tr>
<td>MFB</td>
<td>-0.54</td>
<td>0.13</td>
<td>0.08</td>
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<td>BNMBF</td>
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<tr>
<td>Targets</td>
<td>1.09</td>
<td>0.92</td>
<td>0.85</td>
<td>0.85</td>
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</tbody>
</table>
Results - Nitrogen - Scatter Plots
Results - Nitrogen - Scatter Plots

N OXIDIZED
EMEP
CHIMERE

N REDUCED
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, \( BNMFB_{BD} = BNMFB_{BP} + BNMFB_{BDC} \)
  - \( BNMFB_D \) = 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.
BNMBF TOTAL JUN-SEP (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.

<table>
<thead>
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<th>Metrics</th>
<th>CHIMERE Sulphur</th>
<th>EMEP Sulphur</th>
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<tbody>
<tr>
<td>R</td>
<td>0.55</td>
<td>0.43</td>
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<td>MFB</td>
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<td>NMAE</td>
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<tr>
<td>Targets</td>
<td>0.89</td>
<td>1.09</td>
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Results – Sulphur – Scatter Plots

EMEP

2005

2006

2007

2008

CHIMERE

2005

2006

2007

2008

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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!