Combination of measured and modelling data in air quality assessment in Spain

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INTRODUCTION

The European and Spanish laws oblige to the Governments to provide reliable information about the air quality in Spain every year regarding concentration levels and exceedances of air quality standards. The use of just air quality measurements can provide an incomplete picture of the air quality, as monitoring sites can not cover all the territory. Thus, the use of complementary techniques, such as modelling, is allowed and recommended in many cases. The combination of air quality measurements at stations and validated model estimates is a good choice, due to the accuracy of measurements and the good spatial cover of models.

In this presentation, a methodology to combine measurements from air quality stations and estimates from the CHIMERE model for air quality assessment in Spain is described. The methodology consists of using linear regression and kriging interpolation to correct the model results improving the fit to the observations. It was separately applied to rural and urban conditions, yielding to maps for each case, which were then combined by taking into account the distribution of rural and urban areas in the domain. The results for several pollutants and its application to air quality assessment in Spain are shown and discussed.

METHODOLOGY

Measurements-model combination methodology

Real concentration of an atmospheric pollutant *C* in a station *k* can be expressed as $C_k = M_k + e_k + s_k$

M_k = concentration estimate (i.e., by a dispersion model),

e_k = systematic error of the estimate (i.e., modelling error)

s_k = the inherent error or measurement error.

¿How to reduce the model error e_k, that is, how to correct the model results to provide a best fit to observations and to get a more realistic map of the spatial distribution of pollutant concentrations?.

1) **Linear regression**:

$$C_k = aM_k + b + e_k^{'}$$

a, b = the regression coefficients

e'_k = residual error (includes s_k and the non-solved part of the modelling error (e_k).

This method corrects the concentration estimates by taking into account any influence of the concentration values on them.

2) **Kriging interpolation:**

$$e_k = \sum_{i=1}^{m} \lambda_i e_i + e_k^{''} \qquad \sum_{i=1}^{m} \lambda_i = 1 \qquad C_k^{'} = M_k + e_k$$

λ_i the weights estimated from a variogram in order to minimize the mean-square-error, they range between 0 and 1.

m = number of stations with their residuals to compute e_k.

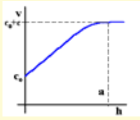
e''_k = kriging error.

The variogram is a function representing how a measured variable varies with distance: $\gamma(h) = \frac{1}{2}\frac{1}{n}\sum[e(x) - e(x+h)]^2$

n = number of stations pairs located to a same distance *h* between them.

Spherical variogram for the values of the concentration differences (or the model residuals) between pairs of stations against the distances between them was used:

$h \le a$ ➔ $\gamma(h) = C_0 + C\left(\frac{3}{2}\frac{h}{a} - \frac{1}{2}\frac{h^3}{a^3}\right)$ $h > a$ ➔ $\gamma(h) = C_0 + C$



Used method:

- to apply the methodology to urban and rural stations separately in order to take into account the different spatial distribution patterns of air pollution concentrations for rural and urban areas obtaining different maps for rural and urban areas.
- to use linear regression and kriging in the case of model residuals for rural stations, and only kriging for urban areas.
- to use spherical variogram for kriging
- to use population density as surrogate indicator for merging urban and rural air pollution maps.

This methodology is applied to the residuals of the CHIMERE model (observation minus model estimation).

Model setup

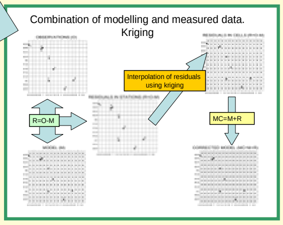
CHIMERE chemistry-transport model (Bessagnet et al., 2004; Hodzic et al., 2005), version 2008c.

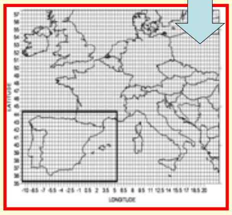
Used for air quality aassessment in Spain since 2004 (Martín et al., 2004, Vivanco et al., 2007).

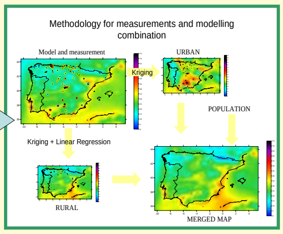
Evaluated using measured air pollution concentrations from Spanish stations (Vivanco et al., 2009a and b) and compared with other models such as CMAQ (Baldasano et al., 2008).

The uncertainty statistics were lower than the maxima established by the EU directives and the EPA criteria.

The MM5 model was the meteorological processor used to input the CHIMERE model. The models were applied to an European domain and then, to an Iberian Peninsula one. Scheme of the model system, boundary conditions, inputs, grid resolution, etc is shown.







RESULTS AND DISCUSSION

Computing concentrations, uncertainty and exceedances probability

CHIMERE run for 2007 ➔ concentrations of SO_2, O_3, NO_2 and PM10 in the Iberian Peninsula and the Balearic Islands.

The methodology to combine measurements and modelling was applied to the residuals of the CHIMERE model computed for the set of air quality stations used for air quality assessment except to the traffic stations.

Maps of average concentrations and the N^{th} higher value at every grid cell, such as $N=Np+1$, where *Np* is the number of exceedances allowed by the European directives for each pollutant.

Uncertainty of the combination methodology based on the uncertainty of the kriging interpolation,

$$\delta_c(x,y) = \sqrt{2\gamma(h)}$$

This uncertainty estimate was used to compute the probability of having more exceedances of limit or target values than allowed by legislation using the approach of Fiala et al (2009).

How does the combination methodology improve the air quality assessment?

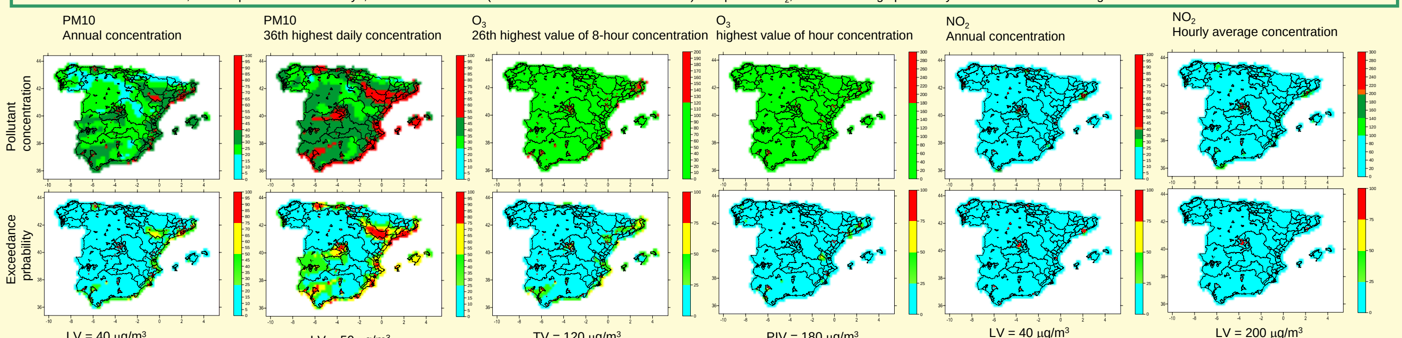
The Maximum Relative Directive Error (MRDE) for the entire domain as the maximum of the Relative Directive Error (RDE) (defined and used in Denby et al. (2010)) found at 90% of the available stations in the Iberian Peninsula and the Balearic Islands is shown in the table. In all the cases the results of the methodology are much better than the model results complying the legal requirements of allowed uncertainty for model techniques used in air quality assessment.

Reference value	MRDE Combination methodology	MRDE CHIMERE Model	Pollutant
Target value 120 μg m^{-3} (eight-hour average)	0.1196	0.1570	O_3
Information value 180 μg m^{-3} (hourly average)	0.2056	0.2510	
Alert value 240 μg m^{-3} (hourly average)	0.1542	0.2064	
Limit value 200μg m^{-3} (hourly average)	0.2315	0.3268	NO_2
Limit value 40 μg m^{-3} (annual average)	0.0549	0.3272	
Limit value 350 μg m^{-3} (hourly average)	0.3288	0.5282	SO_2
Limit value 125 μg m^{-3} (daily average)	0.0804	0.2394	
Limit value 50 μg m^{-3} (daily average)	0.2311	0.6217	PM10
Limit value 40 μg m^{-3} (annual average)	0.1045	0.5224	

Maps for air quality assessment

Maps of air pollutant concentrations and probability of having more exceedances than the legally allowed are shown for O_3, PM10 and NO_2, respectively for 2007.

For ozone, main problems are in the Mediterranean coast, western Andalucia (Guadalquivir valley), some areas in the Cantabric Coast and close to large urban areas (Madrid and Barcelona). In the case of PM10, the risk of exceedances is high in all the Mediterranean Coast, Guadalquivir and Ebro Valleys, Madrid and Asturias (in the north of the Iberian Peninsula). Respect to NO_2, the areas of high probability of exceedances are in large urban areas such as Madrid and Barcelona.



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