EVALUATION OF THE *PRESAXIO* AIR QUALITY FORECASTING SYSTEM: PBL SCHEMES WRF COMPARISON AND AIR QUALITY MODELING VALIDATION

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Abstract: The XIMERE/FUXIMERE project funded by the Galician Ministry of Economy and Industry aims to establish an operational air quality forecasting system, over Galicia (NW of Spain), namely *PRESAXIO* (http://www.presaxio.es). It includes the following models and datasets: WRF-ARW meteorological model (Skamarock et al., 2008), coupled to CHIMERE 2011a+ air quality model (Menut et al., 2010), with NCEP weather forecast as initial and boundary conditions. Detailed regional emission inputs for CHIMERE were prepared (Dios et al., 2012), including E-PRTR and EMEP inventories.

About WRF model performance, four PBL schemes were tested (Yongsei University-Pleim-Chang, Mellor-Yamada-Janjic, Nakanishii-Nino and Hong-Noh-Dudhia). Surface and aloft temperature and wind (speed and direction) against measurements shown that different PBL schemes are recommended depending on primary (SO_2, NO_x) and secondary (O_3) pollution episodes are considered. Finally, the Yongsei University-Pleim-Chang PBL scheme was selected in the operational *PRESAXIO* system, as a compromise solution.

CHIMERE operational results in *PRESAXIO* system was evaluated using DELTA Tool (Thunis et al., 2010) against AirBase air quality data. This CHIMERE implementation provides accurate forecasts of both suburban and rural ozone levels, with small underestimation of primary gas pollutants around specific large point sources, and systematic overestimation of PM10 levels.

Key words: *PRESAXIO air quality forecast, PBL schemes, WRF, CHIMERE, DELTA Tool*

INTRODUCTION

The development and application of operational air quality models is currently an usual practise, thanks to the availability of meteorological and air quality models (i.e. WRF, Skamarock et al., 2008; CHIMERE, Menut et al., 2010), including geophysical databases (i.e. USGS), emissions inventories (i.e., EMEP, PRTR) and large scale numerical weather forecasts (GFS from NCEP). However, over local and regional domains with complex geophysical conditions, accurate high resolution both emissions inventories and numerical weather forecasts are required, in order to reduce the uncertainties associated to the air quality model inputs. In addition, public distribution of the air quality forecasts should be appropriate to both technical air quality management and public spread, also including media.

Different examples of operational air quality forecasts (ESSEM Cost Action 0602) are currently available at Europe. Most of them are designed to cover regional to continental scales and, although their results can achieved up to 1 km^2 of grid resolution, their data input (especially, emissions inventories) are not always adapted to the required accuracy to achieve high resolution results at local and regional scales.

In this work, *PRESAXIO* high resolution regional air quality forecasting system is presented, and their results are evaluated. In order to improve the accuracy of its air quality results, both specific emissions inventories and a numerical weather prediction (NWP) were coupled to CHIMERE air quality model. In addition, different NWPs considering several PBL schemes was tested Air quality forecast was also tested against AirBase air quality data, using DELTA Tool.

PRESAXIO AIR QUALITY FORECASTING SYSTEM

PRESAXIO (Figure 1) includes WRF version 3.2 (Skamarock et al., 2008), configured with 29 or 30 vertical layers (depending on the tested PBL parameterization), and three nested domains with horizontal resolutions of 27, 9 and 3 km^2 (Borrego et al., 2012). CHIMERE model is applied over the two inner domains (Souto et al., 2013). Over the innest domain, a regional high resolution emissions inventory was developed (Dios et al., 2012), combining both point and area sources, and bottom-up & top-down methods.

About the models settings selected, WRF includes: Kain-Fritsch cumulus scheme (outer and medium domain), WSM 3-class microphysics scheme, a RRTM longwave and Dudhia shortwave radiation scheme, and a 5-layer soil model (except with ACM2 Pleim-Xiu PBL scheme, with Pleim-Xiu soil model). A one way nesting option was applied. The NCEP (National Center for Environmental Prediction) GFS analysis data available at a horizontal resolution of 1º x 1º and a 3-hour time resolution were used to input the initial and lateral boundary conditions. Elevation and land cover data were provided by the digital terrain model from the United States Geological Survey (USGS, 2008).

CHIMERE model was set using Vann Leer advection scheme, in order to solve out 20 of 44 chemical species included in the reduced MELCHIOR2 chemical mechanism; aero flag was set in order to activate the aerosols module using 8 bins size distribution; Secondary Organic Chemistry (SOA) are treated using the medium scheme computing. Biogenic emissions data were integrated using the MEGAN model (Guenther et al., 2006) jointly with a meteorological interface to the WRF model. Finally, as initial and boundary conditions, monthly MOZART model results for gases and GOCART model results for aerosols were input.

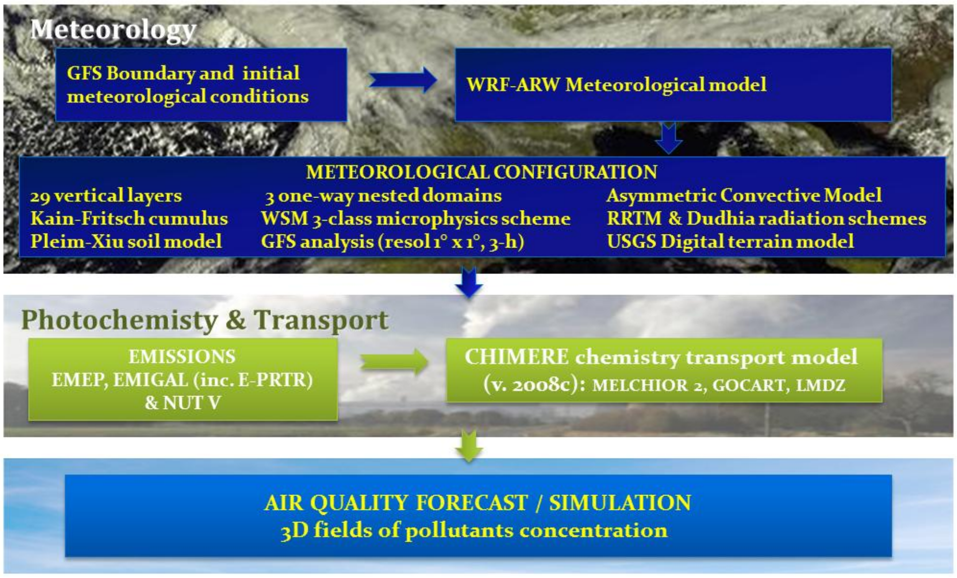

Figure 1. *PRESAXIO* regional air quality forecasting system, with its models and datasets.

RESULTS

Meteorological modeling PBL schemes evaluation

Four numerical experiments for each episode were done, changing the PBL scheme: Yonsei University-Pleim-Chang scheme (YSU), Mellor-Yamada-Janjic (MYJ), Mellor Yamada Nakanishi and Niino Level 2.5 PBL (MYNN) and Asymmetric Convective Model (ACM2). In order to test these PBL schemes, six 3-day air pollution episodes in the NW coast of Iberian Peninsula (IP) were selected (table 1), three of them with high O_3 ground level concentration (glc) and other three with high SO_2 glc.

Table 1. High-ozone and sulfur dioxide episodes selected for WRF model validation in the NW coast of Iberian Peninsula, indicating the maximum O_3 or SO_2 hourly peak.

Episode	Air pollutant	Peak hourly glc ($\mu g/m^3$)
16-18 July 2002	O_3	201.0
19-21 March 2003	O_3	148.0
14-16 September 2003	O_3	193.0
13-15 July 2005	SO_2	304.0
01-03 June 2006	SO_2	324.0
09-11 July 2006	SO_2	174.0

The synoptic weather pattern during the six episodes is clearly anticyclonic and stable, but there are some slight differences between both types of episodes. The rising of surface O_3 levels is associated with a well-defined high pressure center placed to the north of the Iberian Peninsula, over Central Europe or the British Isles (Saavedra et al., 2012a) causing E-SE wind circulation along the northwestern Iberian Peninsula. The synoptic conditions during SO_2 episodes is more variable, but characterized by the Azores anticyclone extending its influence to the Iberian Peninsula and causing E-NE synoptic flux along the same northwestern region.
Comparison of WRF model results with different PBL schemes against wind and temperature measurements from ten surface sites and two operational rawinsondes were done. Considering RMSE and MAGE (Emery, 2001), the most suitable parameterizations for temperature are ACM2 and YSU (Saavedra et al., 2012b). Unlike temperature, the best results for wind speed are achieved by MYNN scheme (Saavedra et al., 2012b), closely followed by YSU scheme. Therefore, YSU PBL scheme can be recommended to simulate high-pollution episodes in this study area, as a compromise between temperature and wind speed performances.

Air quality forecast validation

In order to obtain a representative validation dataset with previously validated air quality measurements, *PRESAXIO* system was run along two different months, July (summertime) and December (wintertime) 2008. Ground level concentrations (glc) of SO_2, NO_2, PM10 and O_3 were considered. DELTA tool v. 2.0 (Thunis et al., 2010) QQ plots show to be very useful in this validation, as follows.

SO_2 glc (Figure 2) is underestimated in the sites located at the NW of the region (especially in summertime), and overestimated in the background EMEP sites (O Saviñao and Noia), at the south. Underestimation is due to the episodic impact of large SO_2 sources in the NW (two coal-fired power plants, Meirama and As Pontes) (Dios et al., 2013a), which was more probable in summer, and cannot be well calculated by the CHIMERE model (even though both were considered as point sources). NO_2 glc (Figure 3) is also underestimated in the NW coast, where important urban areas and also industrial sources are located (Dios et al., 2012). However, in other sites (B2-Louseiras) located close to one of the large coal-fired power plant (Dios et al., 2013b), NO_2 is overestimated. PM10 glc is usually underestimated (Figure 4), but this behavior is not regular. About O_3 (Figure 5), accurate estimations are obtained in the available sites, with overestimation of low glc (at nighttime).

In terms of the application of PRESAXIO results to guarantee the legal glc thresholds, SO_2, NO_2 and O_3 results are considered as acceptable. However, PM10 forecasts are not suitable to be applied. Apart from possible improvements of CHIMERE model PM module, an update of the PM regional emissions inventory is under consideration.

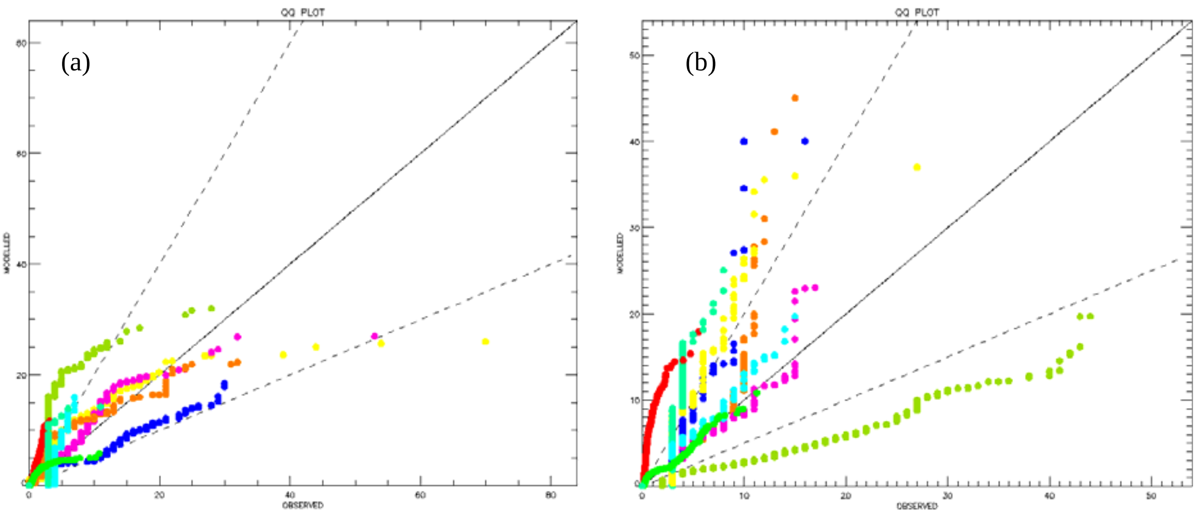

Figure 2. QQ plots of hourly SO_2 glc *PRESAXIO* results over several glc rural sites in (a) July 2008, and (b) December 2008, against the AirBase measurements dataset.

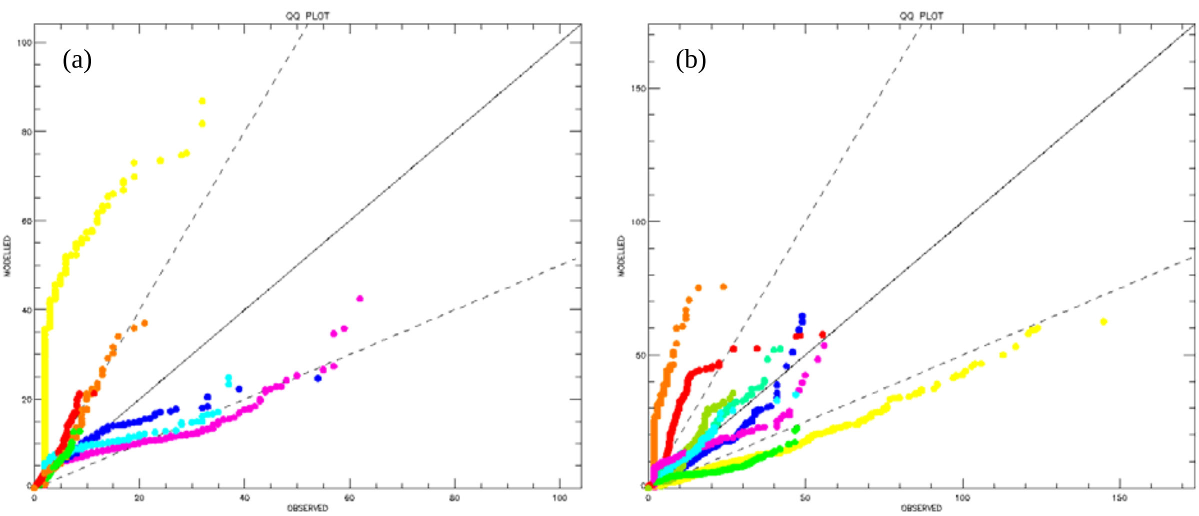

Figura 3. QQ plots of hourly NO_2 glc *PRESAXIO* results over several glc rural sites in (a) July 2008, and (b) December 2008, against the AirBase measurements dataset.

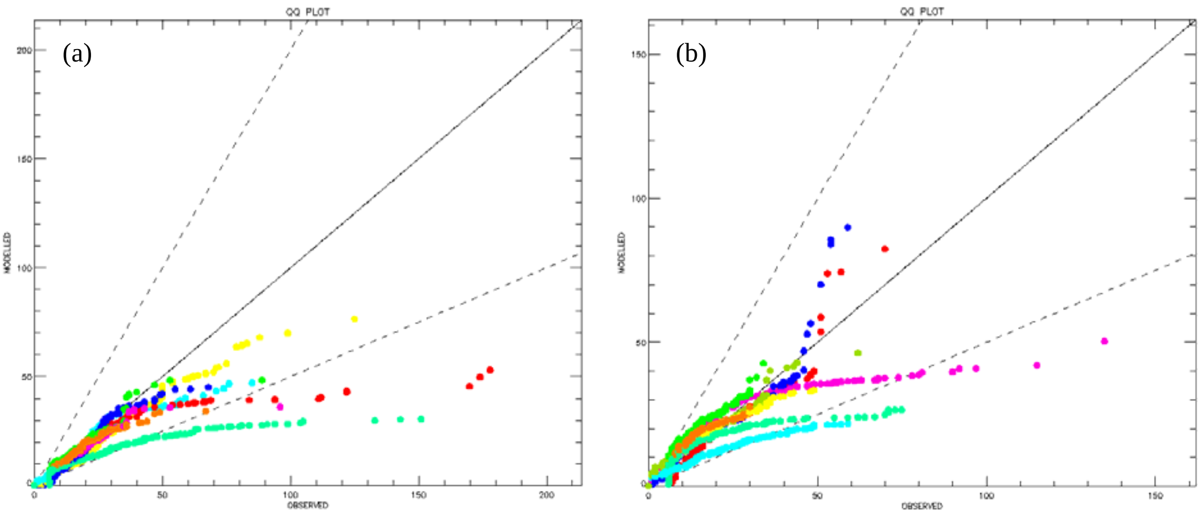

Figure 4. QQ plots of hourly PM10 glc *PRESAXIO* results over several glc rural sites in (a) July 2008, and (b) December 2008, against the AirBase measurements dataset.

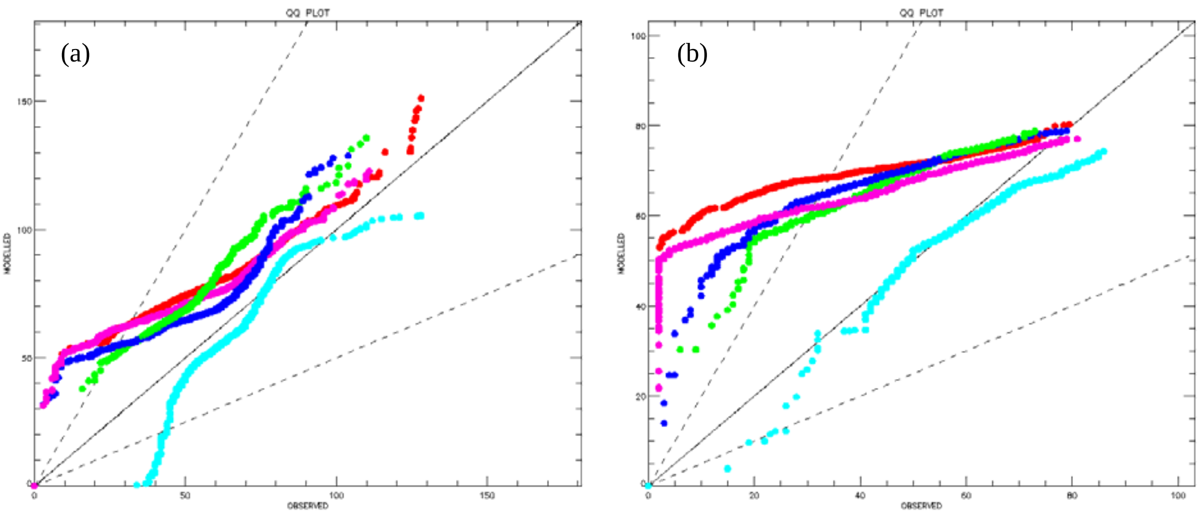

Figura 5. QQ plots of hourly O_3 glc *PRESAXIO* results over several glc rural sites in (a) July 2008, and (b) December 2008, against the AirBase measurements dataset.

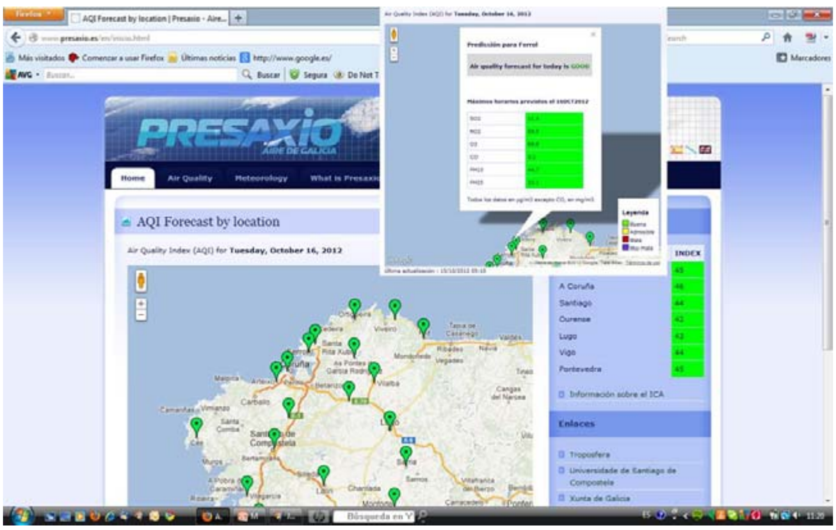

Figure 6. *PRESAXIO* web page, with the Air Quality Index (AQI) forecast. More examples of time series and maps in: www.presaxio.es.

CONCLUSIONS

PRESAXIO operational air quality forecasting system was presented and tested along different periods, in order to evaluate its suitability to provide an air quality forecast to the people. Considering the significance of PBL structure in the results of high resolution air quality modelling, different PBL schemes were tested in WRF model, showing that the best results (compared to both surface and aloft measurements) were achieved using Yonsei University scheme (YSU) scheme. In addition, a two months validation of CHIMERE air quality model was done using DELTA tool and AirBase dataset, showing that SO_2, NO_2 and, especially, O_3 forecasts are suitable to be applied in order to prevent exceedances of their legal glc thresholds. However, PM10 forecasts show an irregular underestimation.

PRESAXIO results are published in a website (www.presaxio.es), both meteorological and air quality forecasting time series and maps, and Air Quality Index (AQI, Spanish Work Group on Air Quality, 2000) (Figure 6), in order to report air quality risks in the region. Also, *PRESAXIO* air quality forecasts are published by the Galician regional government in its website (www.meteogalicia.es), as information to the people.

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