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HOW DIFFERENT AIR QUALITY FORECASTING SYSTEMS (SHOULD) OPERATE OVER PORTUGAL?

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Abstract: Currently three air quality modelling systems routinely operate with high resolution over mainland Portugal for forecasting purposes, namely MM5-CHIMERE, MM5-EURAD and CALIOPE. Each operates daily using different horizontal resolutions, specific physical and chemical parameterizations, and their own emission pre-processors. Bias-correction studies have demonstrated the benefit of using past observational data to reduce systematic model forecast errors. The present contribution aims to evaluate the application of two bias-correction techniques - multiplicative ratio and Kalman filter - in order to improve the air quality forecast over Portugal. Both techniques are applied to the three modelling systems over the full year 2010. Raw and unbiased model results for the main atmospheric pollutants (O₃, NO₂, SO₂, PM10 and PM2.5) are analysed and compared against 18 monitoring stations distributed within mainland Portugal. Statistical analysis shows that both bias-correction techniques improve the raw forecasts skills (for all the modelling systems and pollutants). Despite the applied techniques have different mathematic formulation and complexity level, there are comparable answers for all the forecasting systems. Analysis performed over specific situations, such as air quality episodes, not-validated or missing data reveals different behaviour of the bias-correction techniques under study.

Key words: air quality forecast, modelling systems, bias correction, multiplicative ratio, Kalman filter.

INTRODUCTION

Air quality forecasting is both a challenge and a scientific problem, being one of the requirements of the Air Quality Framework Directive (2008/50/EC) and a key issue of the Clean Air for Europe (CAFE) Programme. The goals of reliable air quality forecasts are obvious: population exposure can be more efficiently reduced and protected by means of information and short-term action plans. For that, European legislation settled ambient air quality standards for acceptable levels of air pollutants that are exceeded every year, in several Member-States (e.g. Portugal), namely for PM10 and ground-level O₃, are being exceeded every year and during long-term periods (<http://www.eea.europa.eu>). Several operational air quality forecasting systems already exist over Europe (<http://www.chemicalweather.eu>). Some of them forecast at the national level as in Portugal. In particular the MM5-CHIMERE (Monteiro et al., 2005), the MM5-EURAD-IM (Elbern et al., 2007) and the CALIOPE (Baldasano et al., 2008a) forecasting systems are advancing our understanding of atmospheric dynamics in Portugal, with several evaluation studies that support the confidence on the these systems (Monteiro et al. 2005, 2011; Baldasano et al., 2008a, 2011; Pay et al., 2010). Nevertheless, air quality forecast modelling, which rely not only on the meteorological prediction but also on a chemical-transport modelling and on highly uncertain emission inventories, are likely to have significant (systematic) model errors (Borrego et al., 2008). In order to improve each model forecast skill, different bias-correction techniques have been applied and examined (e. g. McKeen et al., 2005; Pagowski et al., 2006; Djalalova et al., 2010; Sicardi et al., 2011). The objective of the present study is to examine the efficacy of two bias-correction techniques, multiplicative ratio and Kalman filter methods, to improve the air quality forecasts calculated from the three operational modelling systems available at high resolution over Portugal mainland domain.

THE AIR QUALITY FORECASTING SYSTEMS

There are three air quality forecasting systems operating over Portugal with high resolution. Both MM5-CHIMERE (Monteiro et al., 2005) and MM5-EURAD-IM (Elbern et al., 2007) modelling systems are being applied by the University of Aveiro's research group using an European/Iberian Peninsula coarse domain as boundary and initial conditions for the nested domain over Portugal with a 10x10 km² and a 5x5 km² horizontal resolution, respectively. The MM5-CHIMERE system is operational with daily forecasts available since 2007: http://adamastor.dao.ua.pt/previsao_qar/. The MM5-EURAD-IM is operational for Portugal since 2010, with also daily forecasts in an hourly basis, as a result of a scientific collaboration between the University of Aveiro and the RIU at the University of Cologne. The CALIOPE system (Baldasano et al., 2008a, 2011; Pay et al., 2010), composed by a set of models: WRF-ARW meteorological model, the High-Selective Resolution Modelling Emission System (HERMES) and the chemical transport model CMAQ, provides high-resolution air quality forecast over Iberian Peninsula with a 4x4 km² horizontal resolution and also with an hourly basis (www.bsc.es/calioppe). The three modelling system have different degrees of complexity and spatial resolution. Additional descriptions and their key features can be consulted on the online Model Documentation System (<http://pandora.meng.auth.gr/mds/mds.php>). Since episodic natural of dust outbreaks are frequently observed over all Iberian Peninsula (Basart et al., 2009), and because the representation of these events cannot be well simulated with solely the information of aerosol boundary conditions, the long-range transport of mineral dust from Sahara desert is modelled by the BSC-DREAM8b model (Pérez et al., 2006). The spatial coverage of the air quality monitoring network, together with the background influence and a minimum data collection efficiency of 75% are the criteria used for the monitoring stations selection. As a result, a total of 18 stations (8 rural, 5 urban and 5 suburban) are selected for the present study. Despite the spatial coverage criteria, there is an evident concentration of monitoring stations over the coastal area and the two metropolitan areas of Porto and Lisbon (not shown). Nevertheless, all the regions of Portugal are covered by at least one rural background station.

BIAS CORRECTION

There are several techniques by which bias correction can be applied as mean subtraction (e.g. Wilczak et al., 2006), multiplicative ratio adjustment (McKeen et al., 2005), hybrid forecast (Kang et al., 2008) and Kalman filter (e.g. Djalalova et al., 2010), among others. The bias correction does not try to gain additional insight into model deficiencies or performance neither to correct them artificially, but intends to remove potential errors intrinsic to each model formulation or input data. In

the present study two post-processing methods are used to correct the bias of the three forecasting systems for all the considered pollutants: a multiplicative ratio correction (McKeen et al., 2005) and the Kalman filter method (Kang et al., 2008). Both techniques are site-specific approaches, since they use past ground-based measurements and simulated data at each monitoring site to revise and improve the current hourly forecasts for the entire year of 2010.

The multiplicative ratio correction

The multiplicative ratio correction (RAT) (McKeen et al., 2005) is a simple approach where the corrected concentration with RAT is estimated based on the application of a correction factor to the raw modelled concentration. The correction factor is calculated as the quotient between the additions of observed and modelled concentrations at a particular hour (h) of the n previous days. To estimate the number of previous days (n), Monteiro et al. (2011) tested different training periods and chosen a 4 day training period (n=4; RAT04) as a compromise between having a sufficiently long period to gather adequate statistics, but not too long to mask seasonal variations. According to Tchepel and Borrego (2010), synoptic conditions are characterized by a 3-4 day period, which supports the chosen training period.

Kalman filter

The Kalman filter (KF) is a recursive, linear, and adaptive method that has been used to improve air quality forecast of ground-based O₃ (Kang et al., 2008; Djalalova, et al., 2010; Sicardi et al., 2011) and PM_{2.5} (Djalalova, et al., 2010) concentrations. KF performance is sensitive to the error ratio ($\sigma^2\eta/\sigma^2\varepsilon$) which indicates the way in which the KF responds to the variations in biases at prior steps. There exists an optimal error ratio to generate the best forecast given the forecast modelling system and the dynamic of the study area. The methodology presented in Kang et al. (2008) for the US was followed for estimating the optimal error ratio, which consists in minimizing the RMSE and maximizing the correlation coefficient for all the stations. Due to the similar characteristic of the selected stations, the similar geography where stations are located, and the relatively low extension of Portugal, it was assume that spatial variability of optimal error ratio over Portugal is insignificant to the Kalman filter performance. Therefore, optimal errors ratios are selected for each modelling system and for all the selected stations over the year 2010. Only in the case of O₃, optimal errors ratios are selected seasonality because it was found that corrected O₃ simulation improved when using seasonally varying values.

THE BIAS CORRECTION ASSESSMENT

The evaluation of the different bias-correction approaches applied to the three modelling system is carried out using classical statistical indicators (Borrego et al., 2008; Dennis et al., 2010). The global skills of the bias-correction approaches are represented by means the Taylor diagrams. Additionally, this evaluation is complemented with analysis of the most important critical points of each bias-correction technique find on the air quality forecast of the three modelling systems under study. As an example, Figure 1 shows the Taylor diagrams for O₃, NO₂ and PM₁₀, where is exhibited the observed and modelled standard deviation (SD), the centred root mean square error (CRMSE) and the correlation coefficient (R) in a single point. Together these statistical parameters provide a quick outline of the degree of pattern correspondence among the raw and the unbiased simulated values of each forecasting system and the observed data. O₃ is expressed in maximum daily concentration (O₃ max-1h); NO₂ and PM₁₀ are expressed in daily mean concentrations. Each Taylor diagram shows the annual performance of the two bias-correction techniques, KF and RAT04, applied to the 3 forecasting systems and the corresponding raw modelling systems over all the studied stations.

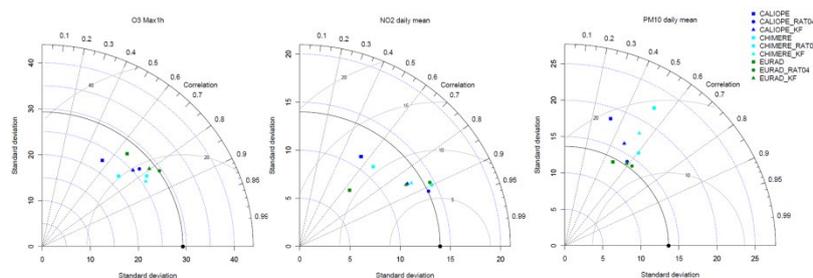


Figure 1: Taylor diagram for each air quality system and for each bias correction technique (KF, RAT04) over all selected stations. (a) O₃ max-1h; (b) NO₂ daily mean; and (c) PM₁₀ daily mean. Black dots are reference point (observed data).

Both KF and RAT04 techniques improve the raw forecasts for all the modelling systems and pollutants, bringing unbiased SD closer to the observed SD than raw modelled SD, reducing errors and increasing correlation coefficients close to the unit. In the case of O₃ max-1h, temporal variability improves in 19-45 % from 0.56-0.81 (raw models) to 0.78-0.86 (KF and RAT04, respectively). The primary pollutants NO₂ and SO₂ (not shown) daily concentrations, demonstrate significant relative improvements compared to O₃, mostly because the original modelling system skills are lower for those species. NO₂ correlation coefficients improve between 30-65% and more than 100% for SO₂ (for both KF and RAT04); and errors decrease also in both cases in ~30-40% (for both KF and RAT04). For PM, improvement after applying both KF and RAT04 are higher with PM_{2.5} (not shown) where correlation coefficients increase in more than 50% (both techniques) reaching values between 0.50 – 0.64. Overall, Taylor diagrams point out that despite the applied techniques have different mathematic formulation and complexity level, there are comparable answers for all of the forecasting systems. There is a slightly superiority of RAT04 technique over Kalman filter in terms of statistical indicator and graphical representation of Taylor diagrams. However, the aforementioned evaluation has the limitation that it is done over all the stations in annual basin and it gives no information whether the unbiased concentrations are correct for the right or wrong reason. Therefore, in order to go more in detail on the skills of bias-correction techniques specific examples of the successes/failures of both techniques are

illustrated following, since it is important to know how RAT04 and KF behave in specific situations, such as air quality episodes and not-validated or missing data, in order to choose the most convenient bias-correction technique to apply on air quality forecast over Portugal. In Figure 3 the hourly observed O_3 concentrations at the CAL station are presented along with the raw CALIOPE outputs and the post-processed KF and RAT04 concentrations during a summer period. This example demonstrates how both KF and RAT04 techniques improve the forecasted O_3 daily cycles, since they agree with the observed hourly variability in both diurnal maximum and night minimum, reducing the persistent overestimation with respect to measurements. Hourly statistical analyses (not shown here) quantify that maximum and minimum annual bias are in the range of $\pm 5 \mu\text{g}\cdot\text{m}^{-3}$ after post-processing with both KF and RAT04. That means a bias improvement of more than 80% in the maximum overestimation (from 40-20 $\mu\text{g}\cdot\text{m}^{-3}$ to less than 5 $\mu\text{g}\cdot\text{m}^{-3}$) for all the system.

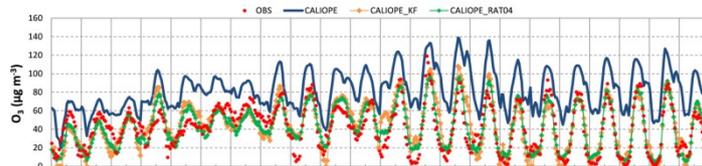


Figure 2: Hourly O_3 time series at the CAL station, estimated by CALIOPE forecasting system (blue) and after the two bias correction techniques KF (orange) and RAT04 (green).

Figure 3 shows PM_{10} time series at FUN station during an air quality episode in August 2010. From August 7th-10th, a desert dust outbreak arrives to Portugal due to a North Africa advection. Raw modeling systems reproduce such episodes thanks to the contribution of the BSC-DREAMb model. After applying bias-correction techniques, unbiased outputs are closer to the hourly observed concentrations. From August 10th to 13th, the wind changes the trajectory to NW (HYSPLIT model results, not shown) and the observed concentrations reach $\sim 170 \mu\text{g}\cdot\text{m}^{-3}$. According to the Portuguese Forest Authority, 9 forest fires occurred during this period in a radius of 100 km from FUN station, where more than 10,000 ha were burned. In the described fire episode both bias-correction techniques do not reproduce the event since the raw modelling systems does not include forest fire emissions. The high bias estimated for this episode generates that both techniques overestimate observed concentration 4 days later after the fire is finished. KF gets closer to the observations faster than RAT04 since KF gradually spreads the error and RAT04 present high sensitivity to the modelled values magnitude.

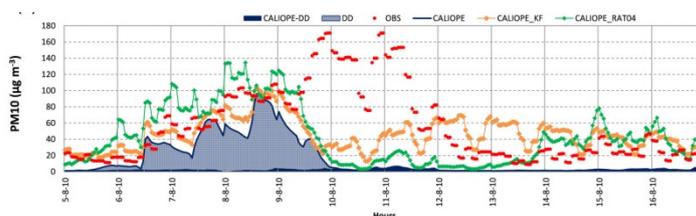


Figure 3: Hourly PM_{10} time series at FUN station for CALIOPE forecasting system (blue line) and the KF (orange) and RAT04 (green) bias correction techniques from August 5th-16th. Area plot shows the modelled desert dust (DD) and anthropogenic contribution (CALIOPE-DD).

Accurate SO_2 forecasts depend on the accuracy in the meteorological patterns, the variability on the sub-grid scale with respect to measured data (Baldasano et al., 2011), and the accurate representation of emissions sources, namely industrial point sources (<http://www.emep.int/>). The Figure 4 illustrates an episode of high SO_2 concentrations at the CHA station, on March 27th from 6:00 to 12:00 where any of the forecast systems were able to predict the observed event. This example demonstrates that both KF and RAT04 produce an error due to high concentrations observed, which is propagated to the same hour during the days after. The propagated error is higher for RAT04 than KF since RAT04 is a simple technique by which simulated and observed data have the same weight. RAT04 applies a correction on the same hour of the next days and if there is no other high concentration during 4 days, the hourly correction factor error will not be reproduced on the 5th day after. On the other hand, the optimal ratio of KF is low (~ 0.04) which means that KF has more confidence on model simulations than observations data. In this sense, the propagated error by KF is less than RAT04 error. In addition, if no other high concentration is recorded, KF error will decrease over the next days, meaning that corresponding bias will be getting closer to 0. The propagation of an error produced by model simulations or observations data (both by a high recorded concentration and by not validated data) is a characteristic of both techniques. This example illustrates that despite the general better performance of RAT04, KF can generate a correction with less error in these specific situations.

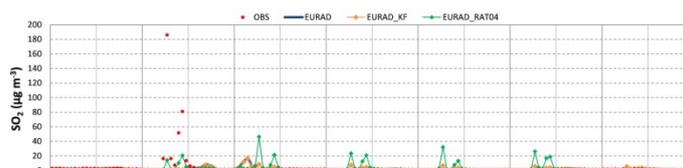


Figure 4: Hourly SO_2 time series at the CHA station, measured and estimated with the MM5-EURAD-IM forecasting system (blue) values and applying the two bias correction techniques KF (orange) and RAT04 (green), from March 26th to April 1st, 2010.

Figure 5 shows an episode registered at the MVE station where the several systems forecasted high SO_2 concentrations that actually did not occur. The figure demonstrates the limitations of the KF technique against high overestimation of the models.

RAT04 technique corrects the raw forecast following the hourly observation with a bias reduction of 80%. This poor performance of KF is related with two facts. First, SO₂ optimal error ratio ($\sigma^2\eta/\sigma^2\varepsilon$) for the 3 models is between 0.13-0.20, higher compared to the other pollutants ratios. When ratio is high, the forecast-error white-noise variance ($\sigma^2\varepsilon$) will be relatively small compared to the true forecast-bias white-noise variance ($\sigma^2\eta$). Therefore, the filter will put excessive confidence on the previous forecast and the predicted bias will respond very quickly to previous forecast errors. Second, KF is a linear and recursive algorithm. KF predicts the future bias with a linear relationship given by previous bias estimate plus a quantity proportional to the difference between the present forecast error and the previous bias estimates. Therefore KF is unable to correct large bias due to model overestimations when all the biases for the past few days have been small.

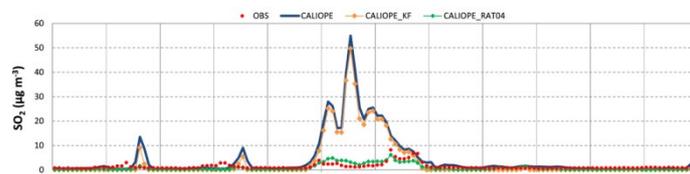


Figure 5: Hourly SO₂ time series at the MVE station for the CALIOPE forecasting system (blue) and the two bias correction techniques KF (orange) and RAT04 (green) from October 25th to 30th, 2010.

The absence of monitoring data is frequently a problem for bias-correction procedures. In case of the RAT04 approach, if there are no measurements, the unbiased outputs will be equal to the raw modelled data. On the other hand, KF has the capacity to learn the behaviour of simulations data relatively to monitoring data, which means that KF is designed to apply the same correction as that estimated for the previous days. Figure 6 illustrates this problem with an example of 2 different periods of absence of measurement data registered at the CAL station. In the first half period (from April 10th to the half of April 14th) KF and RAT04 produce a reasonable corrections with bias values closer to 0. During the periods of April 14th-18th and April 23rd-25th, there are no monitoring data. KF applies the same correction from previous days and RAT04 does not correct the simulated data, taking the same raw modelled outputs. When data start to be available, KF continues to apply the bias correction base on previous days and after four days the recent measurements have an effective effect on bias correction. With RAT04 technique the simulated data is only possible to be corrected after 4 days of data availability.

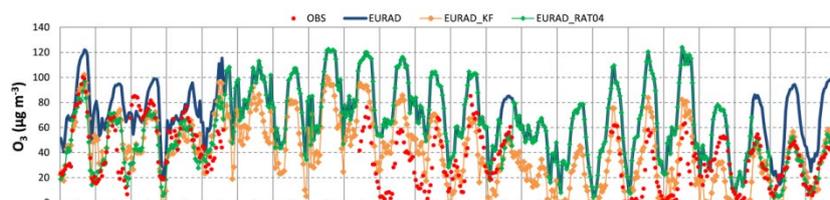


Figure 6: Hourly O₃ time series at the CAL station for MM5-EURAD-IM forecasting system (blue) and the two bias correction techniques KF (orange) and RAT04 (green), from April 10th to May 1st, 2010.

Both techniques are sensitive to not validated data which is a frequent problem for time forecasting mode working. Figure 7 shows an example of not validated data (due to equipment calibration problem), where the time series of SO₂ concentrations at the MVE station present two clear periods of different magnitude values. In this situation both KF and RAT04 correct the raw forecast to agree with observations in the both aforementioned situations. On one hand, KF presents a robust response against a systematic bias. KF gives more confidence to the observations based on persistent systematic bias, and adjusts the background levels, with a transition period of 4 days till the bias is reduced to 0 (orange line). On the other hand, RAT04 tries to adjust background levels in both situations, but produces overestimations during these periods. These instabilities show its sensitivity to high gradient of concentrations and it is a limitation of multiplicative techniques (Wilczak et al., 2006).

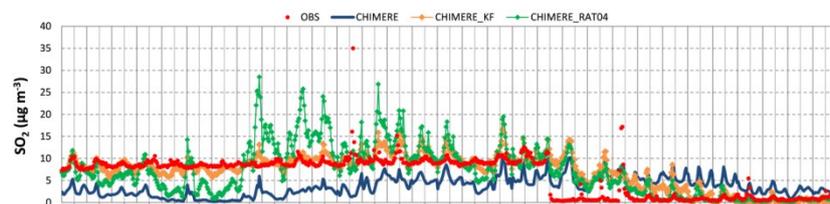


Figure 7: Hourly SO₂ time series at the MVE station for the MM5-CHIMERE system (blue) and the two bias correction techniques KF (orange) and RAT04 (green) from June 3th to July 3th, 2010.

SUMMARY AND CONCLUSIONS

The current work performs an exhaustive examination of two different bias-correction techniques, the Kalman filter method (KF) and a multiplicative ratio with a 4 days training period (RAT04), within their application mainland Portugal domain. Both approaches have been applied to the three advanced forecasting systems operated routinely over Portugal in 2010 – CALIOPE, MM5-CHIMERE and MM5-EURAD-IM. The evaluation is performed for both gas-phase (O₃, NO₂, and SO₂) and particulate matter (PM10 and PM2.5) pollutants. Comparative statistical analysis, based on Taylor diagram, show that both KF and RAT04 techniques improve the raw forecasts skills (for all the modelling systems and pollutants), bringing unbiased SD closer to the observed SD, reducing errors and increasing correlation coefficients close to the unit. Despite the

applied techniques have different mathematic formulation and complexity level, there are comparable answers for all of the forecasting systems. There is a slightly superiority of RAT04 technique over KF in terms of statistical indicator and graphical representation of Taylor diagrams. However, the analysis performed over specific situations, such as air quality episodes, not-validated or missing data reveals different behaviour for KF and RAT04. In the case of O₃ concentrations, both bias-correction techniques are efficient tools to improve simulated O₃ daily cycle remaining bias in the range of $\pm 5 \mu\text{g}\cdot\text{m}^{-3}$. Under desert dust advection from Sahara, KF and RAT04 are able to correct PM10 bias within slightly overestimation of RAT04. Nevertheless, under missed pollution events of short-life (< 2 days), as shown with forest fire or high SO₂ peaks, KF and RAT04 have no efficient corrections of large bias. RAT04 applies a correction on the same hour of the next days and if there is no other high concentration during 4 days, the hourly correction factor error will not be reproduced on 5th day after. On the other hand, the propagation of error in KF is less sharp than for RAT04, since give more confidence to previous persistent bias. This is an advantage of KF under not validated data or missing data since the capability of response is higher than RAT04. One evident disadvantage of KF is when the modelling system presents high overestimations (as shown with hourly SO₂ peaks). KF is unable to correct large bias due to model overestimations since the filter puts excessive confidence on modelled forecast. Both techniques are sensitive to not validated data. The application of the discussed critical points will conduct to a better unbiased model performance and higher accuracy of episodes forecasted.

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