Supplementary Material C : Variability of model performances for the base case

Assessment of the sensitivity of model responses to urban emission changes in support of emission reduction strategies

Bertrand Bessagnet[1], Kees Cuvelier[1,], Alexander de Meij[2], Alexandra Monteiro[3], Enrico Pisoni[1], Philippe Thunis[1], Angelos Violaris[4], Jonilda Kushta[4], Bruce R. Denby[5], Qing Mu[5], Eivind G. Wærsted[5], Marta G. Vivanco[6], Mark R. Theobald[6], Victoria Gil[6], Ranjeet S Sokhi[7], Kester Momoh[7], Ummugulsum Alyuz[7], Rajasree VPM[7], Saurabh Kumar[7], Elissavet Bossioli[8], Georgia Methymaki[8], Darijo Brzoja[9], Velimir Milić[9], Arineh Cholakian[10], Romain Pennel[10], Sylvain Mailler[10], Laurent Menut[10], Gino Briganti[11], Mihaela Mircea[11], Claudia Flandorfer[12], Kathrin Baumann-Stanzer[12], Virginie Hutsemékers[13], Elke Trimpeneers[13]*

Affiliations

1) *European Commission, Joint Research Centre (JRC), Ispra, Italy*
2) *MetClim, Varese, Italy*
3) *CESAM, Department of Environment and Planning, University of Aveiro, 3810-193, Aveiro, Portugal*
4) *The Cyprus Institute, Climate and Atmosphere Research Center (CARE-C), 20 Konstantinou Kavafi Street, 2121 Nicosia, Cyprus*
5) *Norwegian Meteorological Institute, Henrik Mohns plass 1, 0313 Oslo, Norway*
6) *Atmospheric Modelling Unit. Environment Department, CIEMAT - Avda. Complutense, 40, 28040 Madrid, Spain*
7) *Centre for Climate Change Research (C3R), School of Physics, Engineering and Computing Science, University of Hertfordshire; College Lane, Hatfield, AL10 9AB, United Kingdom*
8) *Department of Physics, Sector of Environmental Physics & Meteorology, National and Kapodistrian University of Athens, Athens, Greece*
9) *Croatian Meteorological and Hydrological Service, Ravnice 48, 10000 Zagreb, Croatia*
10) *Laboratoire de Météorologie Dynamique (LMD), Ecole Polytechnique, IPSL Research University, Ecole Normale Supérieure, Université Paris-Saclay, Sorbonne Universités, UPMC Univ Paris 06, CNRS, Route de Saclay, 91128 Palaiseau, France*
11) *ENEA – National Agency for New Technologies, Energy and Sustainable Economic Development, Via Martiri di Monte Sole, 4, 40129 Bologna, Italy*
12) *GeoSphere Austria, Hohe Warte 38, 1190 Vienna, Austria*
13) *Belgian Interregional Environment Agency, Rue Gaucheret 92-94, 1030 Brussel, Belgium*

**Retired with Active Senior Agreement*

Corresponding author : Bertrand Bessagnet : bertrand.bessagnet@ec.europa.eu

Model performances have been evaluated against available background urban, periurban and rural observations (AIRBASE 2022) for the main pollutants either for LT or ST simulations. The bias, root mean square error (RMSE) and the Pearson's spatiotemporal correlation are used for the evaluation (Figure 1). The evaluation Figure 1was performed over a common set of stations over each simulation domain. However the data used to calculate the daily and hourly values are not necessary issued from the same dataset. Indeed, hourly concentration values were uploaded by the modelling teams for ST simulations while daily mean outputs mix ST and LT simulations. The full set of statistical indicators is provided in the supplementary material A. Usually, models perform better for hourly than daily concentrations for ozone due to the model's capability to capture well the diurnal cycle. It is the opposite for PM because the diurnal profile is less pronounced as shown in previous exercises like EURODELTA (Bessagnet et al. 2016). Correlations are usually better for $PM_{2.5}$ than for PM_{10} given the larger differences in the methods to simulate natural coarse particles (dust and sea salts). The variability of correlations for daily ozone concentrations is quite large while for NO_2 the range of the values in the core of the distribution (between the 25th and 75th percentiles) is the narrowest. The root mean square error is very sensitive to the bias. A slight positive bias is in general observed for ozone even if some model results display large negative or positive biases up to respectively -35 µg m^{-3} and +50 µg m^{-3}. NO_2 and PM_{10} are often underestimated while the bias for $PM_{2.5}$ is slightly negative for most models.

The highest correlations (in the range 0.50 – 0.94) for a significant number of $PM_{2.5}$ daily and hourly concentrations are observed for CHIMERE and EMEP for episodes in various cities, such as London, Warsaw, Madrid, Oslo, Berlin, and Prague. Over cities, such as Helsinki for EMEP, London for CMAQ, Athens for CHIMERE and WRF-Chem, the correlation is close to zero for some episodes and even negative.

For ozone concentrations, correlations between 0.83 and 0.86 are observed for some model configurations on hourly basis, such as EMEP for the Brussels and Amsterdam short term simulations. For the LT simulation over Zagreb, ADMS displays a noteworthy correlation of 0.89 with a positive bias of +9.8 µg m^{-3}. Over Athens, Copenhagen and Prague the spatiotemporal correlations for daily values drop to 0 or can be slightly negative for some EMEP or CHIMERE configurations. Over the Po Valley, MINNI shows the highest correlations for hourly concentrations for both LT and ST simulations, 0.79 and 0.76, respectively, on hourly basis, with a positive and negative biases, +5.9 and -1.45 µg m^{-3}, respectively.

In the supplementary material A, an excel sheet provides an histogram overview of statistics using filtered data in the main sheet "Statistics». Athens is the most addressed area by modelling teams emphasizing the large spectrum of model performances. Focussing on the ST episode in summer (Figure 2), WRFNKUA displays a very high positive bias for NO_2 (up to +40 µg m^{-3}) and then a negative bias for Ozone. Other models like CHIMERE or EMEP have a lower positive bias for NO_2 but still a negative bias for Ozone. Correlation for PM_{10} hourly concentrations are very low for all models however looking at $PM_{2.5}$ concentrations the statistics are better with a correlation exceeding 0.5 with a WRF-Chem configuration. For this area a limited number of observation are available in the EEA database (only 18 for the $PM_{2.5}$).

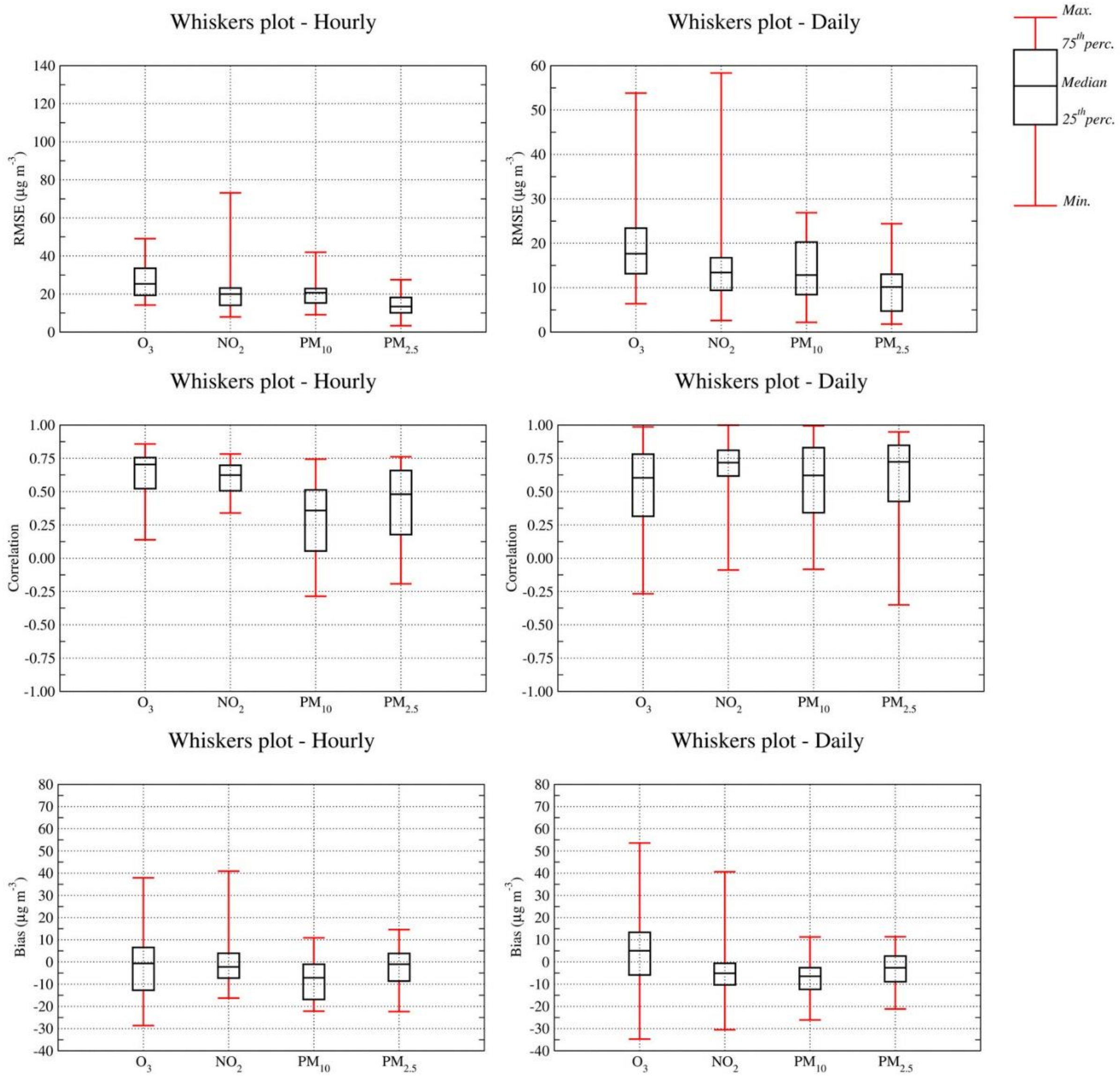

Figure 1: Box and whisker plots of model performances by pollutant (spatio-temporal correlations, Root Mean Square Errors and biases) for short- and long-term simulations on hourly and daily bases.

While uEMEPTAG with its high resolution grid usually displays better performances for NO_2 regarding the bias and then the RMSE, the models fail on the spatio-temporal correlation which is systematically lower compare to the CTM outputs. It is particularly true in Paris (PAR014) where several CHIMERE version operates displaying clearly better correlations particularly the one operated by the CIEMAT with correlation above 0.70 for both $PM_{2.5}$ and NO_2, while NO_2 correlations for uEMEPTAG are close to 0.50. This result is not surprising, an increase of resolution does not automatically provide better results, particularly when the model uses an emission inventory improved by a proxy approach as shown in (Colette et al. 2014).

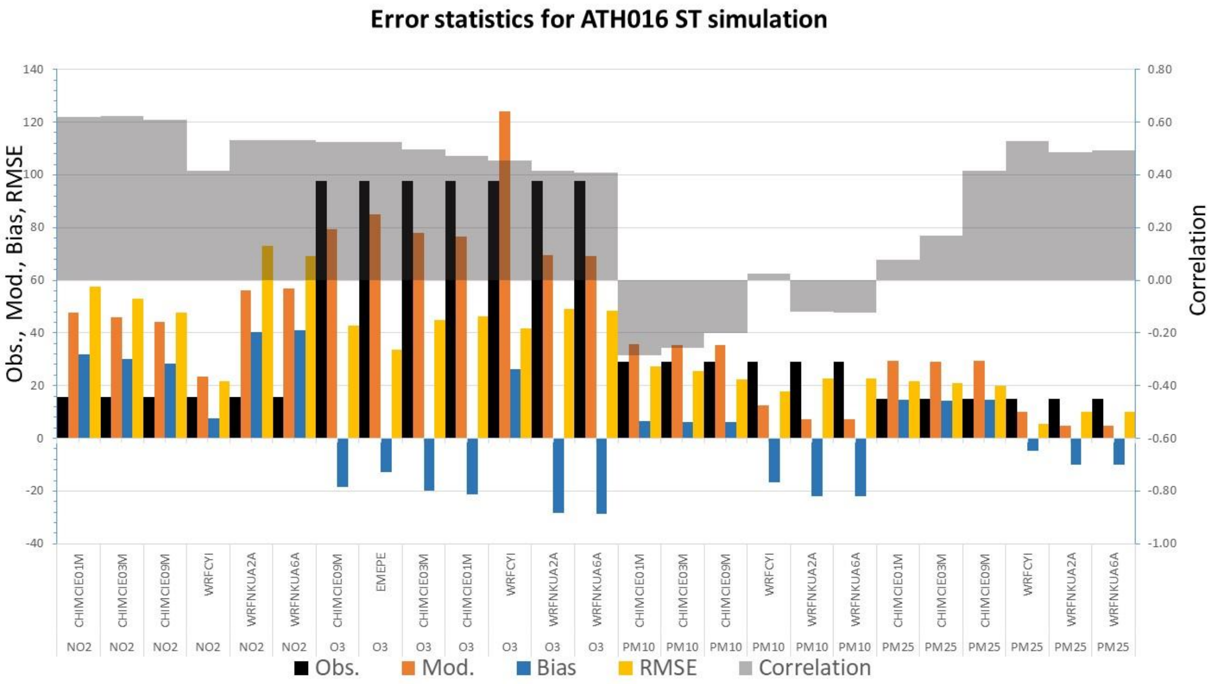

Figure 2: Focus on error statistics over the Athens ATH016 Short Term episode (left y-axis in µg m-3; no unit on right y-axis)

References

AIRBASE (2022) Air Quality e-Reporting (AQ e-Reporting) — European Environment Agency. https://www.eea.europa.eu/data-and-maps/data/aqereporting-9. Accessed 18 Jun 2022

Bessagnet B, Pirovano G, Mircea M, et al (2016) Presentation of the EURODELTA III intercomparison exercise – evaluation of the chemistry transport models' performance on criteria pollutants and joint analysis with meteorology. Atmos Chem Phys 16:12667–12701. https://doi.org/10.5194/acp-16-12667-2016

Colette A, Bessagnet B, Meleux F, et al (2014) Frontiers in air quality modelling. Geosci Model Dev 7:203–210. https://doi.org/10.5194/gmd-7-203-2014