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Evaluation of the chemically speciated particulate matter from a high-resolution air quality modeling system over the Iberian Peninsula

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Particulate matter (PM) is a complex mixture of many compounds, both natural and anthropogenic; that determines its compositions and size. In addition, it is influenced by multiple atmospheric physico-chemical processes that can affect this matter from its release point, as a primary aerosol, or via gas-to-particle conversion processes that give rise to secondary aerosols. Inter-comparisons of European air quality models at regional and urban scales show that models tend to underestimate the observed concentrations of PM10 and PM2.5. Definitely, an accurate representation of the chemically speciated aerosols compounds is required in order to adequately simulate PM concentrations.

The Barcelona Supercomputing Center-Centro Nacional de Supercomputacion (BSC-CNS) currently operates high-resolution air quality forecasts for Europe (12km, 1hr) and the Iberian Peninsula (4km, 1hr) with WRF-ARW/HERMES/CMAQ/DREAM modelling system under the umbrella of the CALIOPE project (http://www.bsc.es/caliope/) and Saharan dust forecasts with BSC-DREAM (http://www.bsc.es/projects/earthscience/DREAM/). In this framework, PM10 and PM2.5 products in both domains are achieved adding the Saharan dust contribution from DREAM (8 bins version) to the anthropogenic output of CMAQ. Furthermore, the CMAQ version used for this modelling system includes the contribution of sea salt aerosols. Eleven different chemical aerosol components can be distinguished, namely nitrates, sulphates, ammonium, elemental carbon, organic carbon with three subcomponents: primary, secondary anthropogenic and secondary biogenic, soil, sodium, chlorine and mineral dust. This study is focused on the evaluation of these aforementioned aerosol compounds from WRF-ARW/HERMES/CMAQ/DREAM over the Iberian Peninsula domain for the year 2004.

The model evaluation with respect to the individual aerosol components has been performed for the domains of study. Albeit PM composition evaluation is presently hampered by the lack of data on particle chemical composition, measurements of PM10 and PM2.5 chemical composition have been made available through the CSIC-IJA for this study. The provided data is spatially and temporally well distributed over eight stations in the Iberian Peninsula and for the whole year 2004, respectively. The model outputs were compared with the daily averages of each aerosol compounds. Statistics and graphics methods are used to describe model skills and weaknesses.

The results of this work demonstrate that evaluation of PM from WRF-ARW/HERMES/CMAQ/DREAM with chemically speciated particulate matter measurements over an entire year (2004) is needed in order to identify which aerosol compounds are not well characterized in the model. PM2.5 sulphate model performance is better than for other species; a large consistency between model and observations was found throughout the year, possibly because sulphate formation chemistry is well understood and the emissions of sulphate precursors are well characterized in HERMES emission model. Carbonaceous aerosol concentration is substantially underpredicted during the entire 2004, most likely due, in part, to a lack of some secondary organic aerosol formation pathways in the model. According to marine aerosol, underestimation of fine Na+ concentration was found, possible due to missed sources of Na+ besides sea salt (mineral dust, surf zone emissions is not included). Fine Cl- concentration is also underestimated because heterogeneous reactions are not taken into account and transfer from PM10 to PM2.5 is not considered. Good correlation for coarse Na+ is found due to its inertness. This kind of information is essential to establish improvement strategies for the prediction of the particulate matter mass over the Iberian Peninsula and to achieve the standards set in European Directives for modelling applications.