Geophysical Research Abstracts
Vol. 12, EGU2010-5279-5, 2010
EGU General Assembly 2010

Chemical composition of particulate matter in Spain: modelling evaluation of the CALIOPE system for 2004

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In the frame of the CALIOPE project, a high-resolution air quality forecasting system, WRF-ARW/HERMES/CMAQ/BSC-DREAM8b, has been developed and applied to the European domain (12km x 12km, 1hr) as well as to the Iberian Peninsula domain (4km x 4km, 1hr) to provide air quality forecasts for Spain (http://www.bsc.es/caliope/). The vertical resolution of the CMAQ chemistry-transport model for gas-phase and aerosols has been increased from 8 to 15 layers in order to simulate vertical exchanges more accurately. Gas phase boundary conditions are provided by the LMDz-INCA2 global climate-chemistry model. The BSC-DREAM8b model simulates long-range transport of mineral dust over the domains under study. The HERMES model system, using a bottom-up approach, was adopted to estimate emissions for the Iberian Peninsula simulation at 4km x 4km horizontal resolution, every hour.

The present contribution describes a thorough quantitative evaluation study performed for a reference year (2004). Model simulations are compared with ground-based measurements from the EMEP and Spanish air quality networks. The speciation of PM10 and PM2.5 from 8 stations of the CSIC-IJA network is analyzed to evaluate the model chemical composition of particulate matter.

Results show that model predictions for relevant gas phase species, such as ozone, are in very good agreement (less than 25% gross error) with observations. Concerning the chemical composition of particulate matter, PM2.5 nitrate and sulphate model predictions are better simulated than for other species; good agreement between model and observations is found throughout the year (correlations around 0.6). Results also show that carbonaceous aerosol concentrations are substantially under-predicted during the entire year, most likely due to a lack of some secondary organic aerosol formation pathways in the model. Good correlation for coarse Na+ is found due to its inertness. Concentrations of fine Na+ are slightly under-predicted due to missing sources of Na+ other than sea salt (e.g., mineral dust). The contribution of paved-road dust resuspension in the coarse fraction of PM10 is shown to have a large impact on urban areas.