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Influence of the PBL scheme on MM5-EMICAT2000-CMAQ high resolution photochemical simulations over a coastal urban site

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The treatment of the evolution and structure of the planetary boundary layer (PBL) in air quality models has important implications for understanding the dynamics of ozone (O_3) and other photochemical pollutants, since meteorological fields developed by meteorological models are used as input to air quality models.

This work analyses the influence of three different planetary boundary-layer (PBL) parameterisation schemes –Gayno-Seaman (GS) (Gayno *et al.*, 1994), Medium Range Forecast (MRF) (Hong and Pan, 1996) and Pleim-Chang (PC) (Pleim and Chang, 1992)– on the predicted ozone and carbon monoxide concentrations fields using the MM5 meteorological model (Dudhia, 1993). The different methods of treating subgrid-scale vertical mixing processes in MM5 would result in different vertical profiles of temperature, cloud cover, and winds, that impact on the concentrations of pollutants in air quality simulations (Ku *et al.*, 2001). Meteorological fields were coupled to the high-resolution EMICAT2000 emission model (Parra, 2004; Parra *et al.*, 2005) and the CMAQ chemistry transport model (Byun and Ching, 1999).

The area of study covers a very complex urban coastal site, the Barcelona Geographical Area, located in the north-eastern Iberian Peninsula. The scenario analysed for an episode of photochemical pollution during May 2002, which is characterised by the absence of large-scale forcing, the development of the Iberian thermal low and compensatory subsidence over the western Mediterranean basin and breeze circulations over the area of study. The PBL remains under 600 m agl due to thermal internal boundary layer formation and large mesoscale subsidence.

Model resolution is 1-km horizontally, and 16 layers of variable thickness in altitude, with the lowest layer being placed at 36m agl. Emissions are supplied by EMICAT2000 including biogenic, on-road traffic, industrial, residential and commercial sources, and fossil fuels burning. These emissions defined the pattern of O_3 precursors on the studied region.

Results of the simulations with the different schemes indicate that modelled daily maximum 1-hr O_3 concentrations appear at different regions of the modelling domain according to the parameterisation of the PBL scheme. In addition, differences in the predicted peak ozone concentrations for a determined hour of the day can be higher than 40 μg m^{-3}; in addition to the differences in the magnitudes of peak ozone, the time of occurrence of maximum concentrations at a given cell or region can differ by several hours.

In order to decide the parameterisation to implement for the area of study and the modelled episode, it becomes essential to characterize the accuracy in the modelling results when assessed against ambient data. Levels of photochemical pollutants were evaluated against measurements from 48 air quality surface stations belonging to the Environmental Department of the Catalonia Government (Spain). The three schemes slightly underestimate ozone concentrations. However, the GS scheme underpredicts the PBL height yielding higher ozone concentrations and a better accuracy in the prediction of 1-hr average concentrations in the Barcelona coastal stations. The MRF and PC schemes overestimate the PBL height in the scenario considered, and therefore the bias values are negative for most air quality stations in the domain.

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