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Global chemical regimes for ozone formation in a global on-line chemical weather prediction model (NMMB/BSC-CHEM)

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Ozone (O_3) production in global chemical models is still an important issue, since O_3 chemistry is inherently nonlinear. Moreover, the kinetics of ozone chemistry and its two main precursors, nitrogen oxides (NO_x) and volatile organic compounds (VOC) represents an important field of uncertainty in atmospheric chemistry. Despite a number of works have been developed trying to evaluate the chemicals regimes of ozone formation by using several indicators based on model species, it is still unclear whether the indicator ratios would show similar behaviour for a wide variety of conditions.

In this study we examine the sensitivity of summertime ozone for the year 2004, its precursors, and its production by running a recently developed on-line chemical weather prediction model at a reasonably high resolution (1x1 degree). The model used, NMMB/BSC-CHEM, is a new fully on-line chemical weather prediction system for meso to global scale applications currently under development at Barcelona Supercomputing Center. The atmospheric driver is the NCEP/NMMB numerical weather prediction model developed at National Centers for Environmental Prediction (NCEP). A gas-phase chemical mechanism has been coupled online with NCEP/NMMB. The chemical mechanism implemented is CB05 coupled with Fast-J photolysis scheme. The dry deposition scheme follows the deposition velocity analogy for gases, and scavenging, mixing and wet deposition for grid-clouds and sub-grid clouds are also considered. The biogenic emissions are computed with the online MEGAN model. The POET emission inventory provides the anthropogenic emissions for the simulations.

Diverse photochemical species derived from the air quality model were used as indicators in order to establish the chemical sensitivity regime existing in different regions of the world. These indicadors include NO_y, NO_z, and O_3/NO_y and O_3/NO_z ratios. Variations in indicator behavior are analytically linked to variations in the O_3 production efficiency per primary radical production. H_2O_2- and HNO_3- derived indicators (e.g. H_2O_2/HNO_3, H_2O_2/NO_y or H_2O_2/NO_z ratios) were also used, albeit they entail higher uncertainties for differencing recent and aged ozone. Finally, the photochemical age (PA) also performed as a good indicator to establish ozone chemical regimes since PA is a useful overall measure of where an air mass is in the aging continuum between fresh NO_x emissions at one end (lowest PA values under 0.2 found for Africa, South America and some emitting areas over populated areas of Europe, North America and Asia), and a depleted background-like condition at the other end (values over 0.8 for remote areas from fresh emissions).