



Modeling ozone production in relation to VOC oxidation and the assessment of 2010 ozone control strategies

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Elevated ozone concentrations are frequently observed during summer in many urban and suburban areas in Europe. In many cases, ozone is rapidly built-up under the influence of strong local industrial and road traffic emissions of precursors. In order to reduce the frequency and intensity of these peaks, the regulation of Volatile Organic Compounds (VOCs) and NO_x emissions was promoted in many European countries, and reductions of about 40% are expected by year 2010. The effectiveness of ozone control strategies has been investigated with 3D air quality models for several European cities through punctual case studies comparing ozone peaks obtained both with present and 2010-projected emissions, on specific polluted days. Anyway, a global understanding of the effects of the proposed emission strategies on ozone can only be reached with a chemical analysis setting up the relationships between precursor emissions, VOC oxidation and ozone production within the anthropogenic air mass.

This paper is based on a 3D-modeling case study of fast ozone production in the South of France. The specificity of this work is to present a quantitative and geographical analysis of the role of the degradation of various VOCs in ozone production, as a function of space, time and precursor emissions. Estimates of the participation of VOCs in ozone production for each grid point of the simulation domain were provided by adding inert tracers of VOC oxidation and secondary species transformation in the

chemical scheme, and plotted against the local ozone production rates and concentrations. The final objective is to determine how much the different VOCs participate in the formation of the ozone plume, and evaluate the efficiency of the 2010 ozone policies proposing VOC emission reductions.

The study proposes modeling case studies of ozone pollution in the Fos-Berre-Marseille area, chosen because of its high density of anthropogenic activities, its strong occurrence of ozone events, and the availability of a large 3D measurement database obtained in 2001 during the ESCOMPTE campaign. Simulations of severe ozone episodes observed during the campaign have been conducted with the CHIMERE eulerian model. A phase of statistic validation of the simulation outputs was then conducted using the 3D database. In a first step, specific VOC degradations and their subsequent ozone production were analysed as model outputs in each grid cell and for each hour of the simulation. The speciation of ozone molecules produced from the several VOC degradation pathways was plotted for the points of high ozone production rates : the results confirm the importance of fast-reacting species such as aromatic compounds and alkenes, but also CO, in regional ozone production. Their respective impact could be quantified for each day of the simulation and each grid point of the domain. Complementary 2D-views showed that the impact on ozone of the various VOCs is differently distributed over the domain and relatively to the ozone plume, reflecting the importance of their source distribution. In a second step, the temporal evolution of modeled ozone production rates along the plume was plotted against VOC degradation intensity. For each day, it allowed to determine the temporal evolution of ozone production from various VOCs during the build-up of high ozone concentrations.

The interpretation of these simulations allowed us to define the VOC species most involved in fast ozone production over the domain, but above all to spatialize their impact on ozone with regards to fast ozone production areas. The objective was to characterize the effectiveness of their emission control with regards to the VOC reductions planned for 2010. Projections of 2010 emissions taking into account the european legislation have been carefully elaborated within the frame of this work. Simulations are now being conducted with this set of emissions. Further work will concentrate on the comparison between simulations with present and 2010 emission inventories, in order to lighten the way the emission strategies may influence ozone production, and finally to propose optimized emission strategies.