Modelling the aerosol mass formed in a smog chamber under different VOCs/NOX conditions

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The impact of atmospheric aerosols on human health is an important issue nowadays. As a consequence of the growing presence of these particles in urban and rural areas, new legislation has been established during the last years in order to regulate their concentration in the atmosphere. Among these particles, secondary organic aerosols (SOA) formed from the oxidation of some anthropogenic volatile organic compounds (VOCs) such as benzene, toluene or xylenes have a great impact in urban areas, as these VOCs are common pollutants produced by city traffic. The concentration of SOA is highly related to the relative concentration of VOCs and NOX in the atmosphere, and therefore the control of the emissions of these pollutants seems to be a suitable control strategy to reduce SOA formation. The evaluation of these strategies can be carried out with air quality models, by creating different VOCs-NOX scenarios.

In order to evaluate the sensitivity of the CMAQ 4.7 air quality model to different VOCs and NOX concentrations, some experiments were performed in the EUPHORE smog chamber (Valencia, Spain). In these experiments, the SOA formation from a mixture of anthropogenic VOCs (octane, toluene, o-xylene and 1,3,5-trimethylbenzene) in the presence of an oxidant agent (nitrous acid, HONO) was studied under different VOCs/NOX ratios. These ratios were selected in the range of 6-30 VOCs ug / NOX ug. A base case experiment with fixed VOCs mixture and HONO concentrations was designed. Increments and decreases of these concentrations were studied on the rest of the experiments presented. Aerosol concentration in the chamber was measured with a tapered element oscillating monitor (TEOM), while single and coupled to mass spectroscopy gas cromatography (GC and GC/MS), as well as Fourier transform infrared spectroscopy (FTIR) were used to measure VOCs and HONO concentration.

Simulations were performed with a box model version of the CMAQ model, where only gas phase chemistry and aerosol formation were considered. Two gas phase chemical mechanisms were used (CB05 and SAPRC99) coupled with an aerosol formation module (AERO5).

A general overprediction is observed in the SOA mass formed predicted by the box model simulations for all the experiments. However, the SOA formation response of the VOCs mixture to the different VOCs/NOX ratios simulated by the model generally keeps a relation with the experimental SOA measured in the chamber.