Benefits of cross modelling and field measurement approaches on the evaluation of SOA distribution: a case study in Grenoble, France

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Organic Aerosols represent a major fraction of particulate matter in ambient air, that influence significantly the climate and air quality. Their concentration and composition show a large seasonal and regional variability. Primary emission sources have been widely studied, and are now well known and apportioned. VOCs (Volatile Organic Compounds) can undergo photo-oxidation reacting with light and oxidants like OH, NO_3, O_3, producing less volatile compounds that, through coagulation or nucleation, can form Secondary Organic Aerosols (SOA), which account to a significant part of total OA. To date, air quality models does not succeed to well simulate the SOA fraction in the PM concentration forecasts.

The aim of this work is to evaluate the benefit of the combination of field measurement and modelling on the evaluation of the SOA distribution. Final goal is to improve models for the prediction of SOA formation and contribution in the ambient air.

Aerosol filter samples have been collected at the urban station of "Les Frenes" in Grenoble (France) in 2013 every third day for one year and already included a large aerosol chemical characterization (Tomaz et al. 2016). The samples were extracted by QuEChERS (Quick Easy Cheap Effective Rugged and Safe) (Albinet, Tomaz, and Lestremau 2013) and and analyzed by GC-MS after derivatization with MSTFA+1%TMCS. Quantification of SOA markers (e.g. SOA-Biogenic: pinic acid, pinonic acid, 2-methylerythritol, β-caryophyllinic acid, MBTCA, SOA-Anthropogenic: DHOPA, DHOBA, SOA-PAH: hydroxypyrene, 4 – nitro – 1 - naphtol, 1 acenaphtenol, SOA-Biomass Burning: methyl-nitrocathecols) was done using native standards.

The estimation of the SOA (or SOC) contribution from individual precursor was performed using the SOA tracers method proposed by (Kleindienst et al. 2007). This approach uses ratios obtained by chamber studies between markers produced and the amount of precursors introduced.

The chemistry-transport model CHIMERE (Menut et al. 2013) was used for SOA distribution modeling, taking both anthropogenic and biogenic markers into account. For selected SOA marker, the atmospheric formation pathway was sought in the literature and inserted in the model. Kinetic data were taken from The Master Chemical Mechanism database (National Centre for Atmospheric Science, Universities of Leeds and York). The simulation was performed over Europe and at regional scale (Figure 1)

The novelty of in this work relies in the synergy between the analysis of field data and the improvement of the model. The results from one-year campaign measurement was compared for the first time to the output of modeling simulation on a regional scale. This kind of approach is required in order to get an overview of the SOA distribution at a local scale, since the actual concentrations are often underestimated. This is the first step towards a better understanding of the processes occurring in the atmosphere in order to improve atmospheric chemistry models and efficiency of air quality control policies.

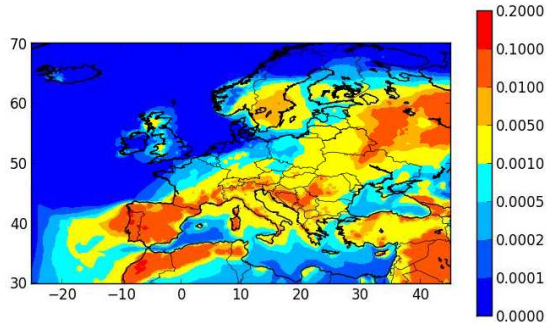

Figure 1. Map of distribution of Pinonic acid (ng/m^3) all over Europe between 07-09 July of 2013, simulated by CHIMERE

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