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Particle Formation in Photo-oxidation Experiments with 2-Aminoethanol (MEA)

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2-Aminoethanol (MEA, NH₂CH₂CH₂OH) is a widely used compound for post combustion CO₂ capture in modern Carbon Capture Systems (CCS). The capture process entails emissions of substantial amounts of amines to the atmosphere. Quantitative knowledge about the atmospheric fate of MEA, including partitioning to particles and droplets and contribution to formation of new particles, is prerequisite to an Environmental Impact Assessment of amine-based CO₂-capture. Despite the need for reliable data only few studies on the atmospheric photo-oxidation of MEA exist to date. The atmospheric photo-oxidation of MEA was studied at the European Photochemical Reactor, EUPHORE, in Valencia (Spain). The photochemical degradation of MEA was monitored in situ by FT-IR and on-line by PTR-TOF-MS, and the formation of particles by SMPS and AMS on-line instruments and filter sampling followed by analysis with LC/HRMS(TOF). The experiments were carried out under varying NOx conditions and initial MEA gas phase mixing ratios ranged between 100 and 700 ppbv. The photo-oxidation of MEA was found to give raise to ozone and significant formation of particles. Aerosols were formed immediately after the exposure of the chamber to sunlight with number concentrations ranging up to 10⁴ particles/cm³. Monitored particle number size distributions revealed steep growth curves during the experiments and total aerosol mass concentrations increased up to 230 μ g/m³. The aerosol mass spectrum is found to be quite different from that of the pure (stoichiometric) ethanolammonium nitrate salt and contains a small fraction of higher molecular weight organics, consisting of C3 and C4 fragments. The high molecular weight organic fraction increased throughout the course of the experiment, but contributed only 1.1% of the total aerosol mass. This is in line with the work of Murphy et al. (2007) who indicate that the mass yield of non-salt aerosol during photo-oxidation experiments with aliphatic amines is in general low. The recently developed sectional aerosol dynamic model MAFOR was applied to investigate the mass closure for MEA during photo-oxidation experiments. MAFOR has been extended in the frame of this study to include 1) chamber specific losses of gases and particles, 2) chamber specific sources, 3) monitored time series, 4) MEA photo-oxidation chemistry, 5) condensation of a low-volatile MEA oxidation product to existing particles, 6) condensation of a gas phase acid-base equilibrium reaction product, and 7) nucleation involving MEA and nitric acid. According to model simulations, MEA is to a large extent degraded by chemical reaction with the OH radical (30-50%), a substantial amount of the injected MEA amount (40-60%) is converted into particle mass (gas-to-particle conversion) during the photo-oxidation experiments, while about 10-30% of the initial MEA amount is lost to the walls or by dilution through replenishment flow.