

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



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1. Introduction

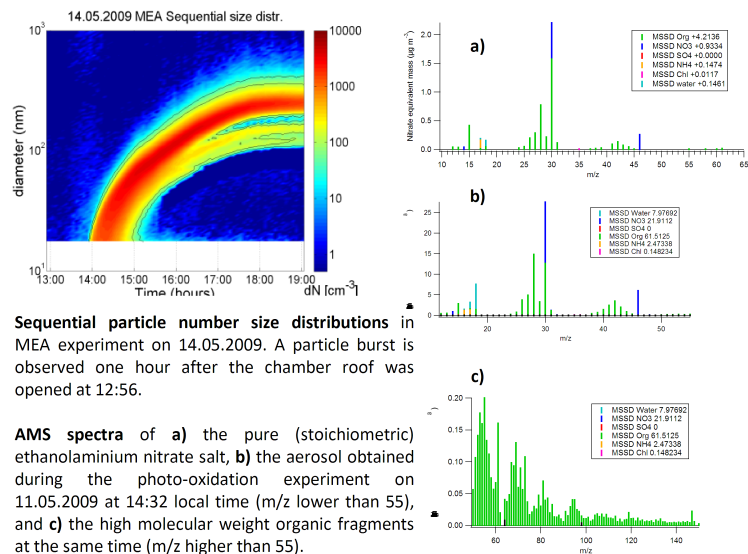
2-Aminoethanol (MEA, $\text{NH}_2\text{CH}_2\text{CH}_2\text{OH}$) is a widely used compound for post combustion CO_2 capture in modern Carbon Capture Systems (CCS). The capture process entails emissions of substantial amounts of amines to the atmosphere. Quantitative knowledge about the atmospheric fate of MEA, including partitioning to particles ([1],[2]) and droplets and contribution to formation of new particles [3], is prerequisite to an Environmental Impact Assessment of amine-based CO_2 -capture. Despite the need for reliable data only few studies on the atmospheric photo-oxidation of MEA exist to date ([4],[5]). The atmospheric photo-oxidation of MEA was studied at the European Photochemical Reactor, EUPHORE, in Valencia (Spain).



Dome of the EUPHORE chamber B

3. Particle Formation

The aerosol mass spectrum is found to be quite different from that of the pure (stoichiometric) ethanolanmonium nitrate salt and contains a significant fraction of higher molecular weight organics, consisting of C3 and C4 fragments. Recent lab experiments using soft ionization AMS indicate that the high MW organics may contribute up to 15-20% of the total aerosol mass. This contrasts with the work of Murphy et al. [2] who show that the mass yield of non-salt aerosol during MEA photo-oxidation experiments is only 2-3%.



2. Method Description

The recently developed sectional aerosol dynamic model MAFOR [6] was applied to investigate the mass closure for MEA (see Table at bottom). 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], 5) condensation of a low-volatile MEA oxidation product to existing particles, 6) condensation of a gas phase acid-base equilibrium reaction product:

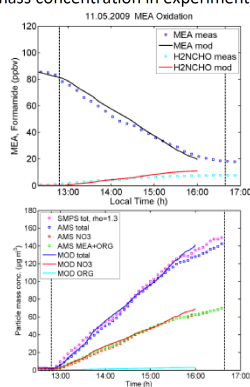
$\text{MEA(g)} + \text{HNO}_3(\text{g}) \rightleftharpoons \text{MEANO}_3(\text{s})$ (R1)
and 7) nucleation involving MEA and nitric acid. The relative contribution of loss processes to the overall decay of MEA in the experiments was derived by scaling five model fit parameters (HONO wall source strength, condensation and nucleation of MEA-HNO_3) to simultaneously match the measured gas phase concentrations of MEA, formamide, and ozone as well as total and nitrate aerosol mass concentrations.

Mass balance of MEA: chemical reaction, conversion to particulate phase and wall loss (including dilution loss).

Experiment Date	Chemical reaction (%)	Particle conversion (%)	Wall loss (%)
10.05.2009	51	21	28
11.05.2009	31	36	33
14.05.2009	42	5	53
15.05.2009	16	13	71

4. Models vs. Measured Results

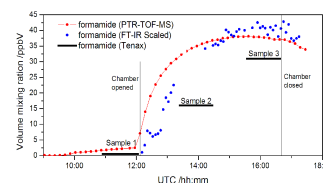
Example for mass balance determination. Model fit to measured time series of MEA, formamide and aerosol mass concentration in experiment on 11.05.2009.



Gas phase product formamide measured by PTR-TOF-MS, FT-IR and by Tenax/GC-MS in the experiment on 15.05.2009

Several parallel measurement techniques have been used to monitor gas phase compounds and particles.

Instrumentation at Euphore	
SMPS	Number size distribution
TEOM	Total mass concentration
AMS	Particle size distribution and chemical composition
PTR-TOF-MS	MEA and gas phase products
FT-IR	MEA, NH_3 , formamide
DNPH, Tenax filters (GC-MS, LC-MS)	MEA, formamide, gas and particulate products



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