Geophysical Research Abstracts
Vol. 18, EGU2016-16477, 2016
EGU General Assembly 2016

Advanced modelling of the multiphase DMS chemistry with the CAPRAM DMS module 1.0

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Oceans are the general emitter of dimethyl sulphide (DMS), the major natural sulphur source (Andreae, 1990), and cover approximately 70 % of earth's surface. The main DMS oxidation products are SO_2, H_2SO_4 and methyl sulfonic acid (MSA). Hence, DMS is very important for formation of non-sea salt sulphate (nss SO42-) aerosols and secondary particulate matter and thus global climate. Despite many previous model studies, there are still important knowledge gaps, especially in aqueous phase DMS chemistry, of its atmospheric fate (Barnes et al., 2006).

Therefore, a comprehensive multiphase DMS chemistry mechanism, the CAPRAM DMS module 1.0 (DM1.0), has been developed. The DM1.0 includes 103 gas phase reactions, 5 phase transfers and 54 aqueous phase reactions. It was coupled with the multiphase chemistry mechanism MCMv3.2/CAPRAM4.0α (Rickard et al., 2015; Bräuer et al., 2016) and the extended CAPRAM halogen module 2.1 (HM2.1, Bräuer et al., 2013) for investigation of multiphase DMS oxidation in the marine boundary layer. Then, a pristine ocean scenario was simulated using the air parcel model SPACCIM (Wolke et al., 2005) including 8 non-permanent cloud passages - 4 at noon and 4 at midnight. This allows the investigation of the influence of deliquesced particles and clouds on multiphase DMS chemistry during both daytime and nighttime conditions as well as under cloud formation and evaporation. To test the influence of various subsystems on multiphase DMS chemistry different sensitivity runs were performed. Investigations of multiphase chemistry of DMS and its important oxidation products were done using concentration-time profiles and detailed time-resolved reaction flux analyses.

The model studies revealed the importance of aqueous phase chemistry for DMS and its oxidation products. Overall about 7.0% of DMS is effectively oxidised by O_3 in the aqueous phase of clouds. The simulations revealed the importance of halogen and aqueous phase chemistry for DMS and its oxidation products. Overall halogen compounds contribute with 71% to DMS oxidation with gaseous Cl (23.6%) and BrO (46.1%) as main oxidants. The conversion efficiency of DMS to SO_2 in the gas phase was simulated between 0.2, 0.27 and 0.6 for the full pristine ocean scenario run, a simulation without considered halogen chemistry and a simulation without treated aqueous phase DMS chemistry, respectively. Furthermore, the studies indicate that the conversion efficiency of DMS to MSA is strongly related to DMS oxidation by BrO and treating of aqueous-phase DMS chemistry. The MSA yield for different sensitivity runs was simulated between 0.01 and 0.47. The lowest yield is reached treating only gas phase chemistry of DMS. Moreover, the simulation with the whole mechanism indicate that multiphase DMS oxidation produce as much MSA as sulphate leading to strong implications for nss-$SO_4{}^{2-}$ aerosol formation, activation to cloud condensation nuclei and cloud albedo.

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