Halogen Production from Aqueous Tropospheric Particles:
A Modelling Study

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Introduction
Halogen play an important role in chemical processes in the marine boundary layer. Halogens-containing compounds are released from sea-salt aerosols and then destroyed photchemically to form very reactive halogen atoms. Up to now only studies on the topic of activation of halogens from sea-salt particles were performed to understand the high amounts of halogen radicals in the gas phase. But there is still a large uncertainty in explaining the processes leading to halogen activation. Within this project the production and release of halogens from cloud droplets into the gas phase is investigated. Although the concentration of halides in cloud droplets is smaller than in sea-salt particles the concentration of activated halogens from cloud droplets can reach similar levels. For describing this process a very complex mechanism (RACM, CAPRAM 2.4 (MODAC-mechanism)) is used and an additional module (HALOGEN1.2) for the explicit description of halogen-solution chemistry was developed.

Mechanism and parameters

Conditions of the cloud
(for box modeling)
(taken from CAPRAM 2.4 (MODAC-mechanism))

Introduction

Mechanism and parameters

Reactions in the gas phase

Phase transfer processes (as proposed by Schwartz, considering K_{ij, k, l, m})

Aquaplan phase (inversible reactions, X=B or Cl)

Equilibrium
dissociation of HBr, HBrO, HBrO_{2}, HClO
formation of trihalide anions: BrCl, BrCl_{2}, BrCl_{3}
hydrolysis of BrCl, Cl\_2, Br\_2
reactions of the oxoalum compounds BrO\_2, BrO\_3, HBrO_{2}, and HBrO (FKN mechanism; Field et al., 1986)

Table 1: Comparison of halogen atom concentrations in either phase for the maritime and polluted scenario

Conclusion

Although the concentration of halides in cloud droplets is lower compared to that in sea-salt particles the amount of activated halogen is the same order of magnitude.

For the maritime case 10 molecules of Br\_2 and 10 molecules of Cl\_2 are activated.

Chemistry of radicals is important for the release of halogen compounds into the gas phase.

Direct phase transfer of Cl\_2 and Br\_2 is possibly the main source of the halogen radicals in the gas phase.

Activation processes from cloud droplets are different between clean and polluted air masses.

Outlook

calculations with different ionic strengths of halogen containing compounds

development of a module considering DMS oxidation

References


