Modelling Calculations of Gas Phase and Aqueous Phase Chemistry in the Troposphere

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The tropospheric chemistry is described with a box model containing gas and aqueous phase chemistry. The gas phase chemistry bases on the RADM2-mechanism by Stockwell, the liquid phase chemistry is represented by the chemical aqueous phase radical mechanism (CAPRAM). In the calculations 142 aqueous phase compounds are considered, including C_1 und C_2 organic aliphatic compounds, radicals like SO_4^-, NO_3, Cl_2^- and peroxyl radicals. In the model three scenarios, for the marine, urban and rural environment are taken into account. Initial concentrations of the trace gases are taken from Zimmermann and Poppe, the data for the transition metal ions are taken from Matthijsen. The simulations are performed for three days.

The aqueous phase mechanism includes 240 aqueous phase reactions, six photolysis and 17 Henry-equilibria. The uptake processes of eight compounds (OH, NO_3, O_3, CH_3O_2, CH_3O_2H, N_2O_5, H_2O_2 and HO_2) are calculated by means of the resistance model by Schwartz, because their solubility is high, so that they don't reach a thermodynamic equilibrium. Therefore the resistance model takes into consideration diffusion processes in the liquid and gas phase, the uptake coefficient γ, the effective droplet diameter and the mass accomodation coefficient α are used.

The results of the calculations make clear the influence of the aqueous phase to the tropospheric chemistry. Predicted concentrations over three days of some radicals will be presented. The most important sinks and sources for several important species during the day and the night will be discussed.