Geophysical Research Abstracts, Vol. 7, 04450, 2005
SRef-ID: 1607-7962/gra/EGU05-A-04450

SPACCIM Simulations of the Multiphase Chemistry Occurring in Orographic Hill-Capped Clouds

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The parcel model SPACCIM (Spectral Aerosol Cloud Chemistry Interaction Model / Wolke et al., 2005) has been applied to investigate the effect of multiphase cloud processing of tropospheric aerosol particles and trace gases resulting from a passage through an orographic cloud at Mt. Schmücke (Thuringia, Germany) during the joint research project FEBUKO. The applied model includes a complex microphysical and a detailed multiphase chemistry model with about 261 gas phase and 776 aqueous reactions. The chemical multiphase model incorporates a detailed description of the inorganic and organic multiphase chemistry based on time-dependent size-resolved aerosol/cloud spectra. The data measured at the upwind site provided the basis for the chemical and physical model initialisation under real environmental conditions. Simulation results have been compared to experimental cloud water composition data at Schmücke summit site as well as gas and aerosol measurements at downwind site in order to interpret the experimental data and to evaluate the model results. To this end, a detailed analysis of the chemical multiphase system was performed including source and sinks studies with special emphasis on multiphase phase oxidants and S(IV) to S(VI) conversion. Furthermore, in-cloud oxidations of organic compounds have been studied focused on important C2 and C3 oxidation subsystems. This modelling study shows that the observed multiphase chemistry is strongly affected by dynamic microphysical processes. Furthermore, a significant cloud condensation nuclei modification with sizes up to about 400 nm, mass productions up to about 0.7 μg m^{-3} and acidification caused by cloud processing was identified. The concluding comparison between model results and experimental findings at summit and downwind site shows quite

good agreements. However, for organic compounds with low solubilities the cloud water measurements show considerably higher concentrations than expected from both (i) their Henry solubilities and (ii) the complex multiphase modelling as performed by the model.