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Simulation Tools for the Lagrangian Modelling of Joint Microphysical and Chemical Cloud Processes

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Multiphase processes, such as the uptake of gases and radicals by clouds or the production of gas phase halogens from particulate halides, are of increasing importance for the understanding of the tropospheric system. Phase transfer and chemical reactions modify the concentrations of stable compounds and oxidants in either phase. Simulation tools are presented which allow the modelling complex multiphase chemistry together with microphysics. The description of both components is given for a fine-resolved particle/drop spectrum. Two modelling approaches are presented. The parcel model SPACCIM (Spectral Aerosol Cloud Chemistry Interaction Model / Wolke et al., 2005) couples two independent models with different options for the interaction between the chemistry and the microphysics models. In the second model water vapour and trace gases on one side and solutes and water on the other side are treated in a unified way. Water and solutes are parts of an internally mixed particle population which is discretized in mass space with respect to the total mass of the particles. The simulation environment allows to configure a lot of different scenarios by changing the chemical mechanism in the gas and particle phase, the dry particle composition and number distribution and the meteorological conditions.

A short overview will be given about the numerical methods used which utilize the special structure of the problem. It is shown that the numerical effort increases only linearly with the size of the problem (number of species in the gas and particle phase, number of section in particle mass space).

Both models are applied to the FEBUKO experiment, a measurement campaign to characterize an air parcel during a passage over the mountain Schmücke (Thuringia,

Germany). The sensitivity of simulation results against variations in the particle/droplet size resolution, the coupling type and numerical control parameters is discussed.