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SPACCIM model studies on the multiphase processing of tropospheric aerosols

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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 processing of tropospheric aerosol particles and trace gases based on more realistic meteorological non-permanent cloud model scheme. The applied model includes a complex microphysical and a detailed multiphase chemistry model. The applied multiphase chemistry mechanism with about 1100 processes consists of an extended version of the gas phase mechanism RACM-MIM2 (Karl et al., 2006) coupled to the detailed aqueous phase mechanism CAPRAM 3.0i (Herrmann et al., 2005). The chemical mechanism incorporates a detailed description of the multiphase chemistry based on time-dependent size-resolved aerosol/cloud spectra. The model was initialised with chemical and physical aerosol data (Poppe et al., 2001) for three different atmospheric conditions (urban, remote, marine). Simulations were carried out for a meteorological scenario including 8 cloud passages and an intermediate aerosol state at a 90 % relative humidity level by neglecting the effects of non-ideal solutions. Simulation results have been analysed including time resolved source and sinks studies focused particularly on multiphase phase radical as well as non-radical oxidants and multiphase oxidations of C_2–C_4 organic compounds. The model studies shows significant effects of multiphase cloud droplet and aqueous aerosol interactions on the tropospheric oxidation budget for polluted and remote environmental conditions as well as influenced VOC's oxidation due to the changed oxidation budget. Furthermore, the simulations implicate the potential role of deliquescent particles to act as a reactive chemical medium due to the in-situ aqueous phase production of radical oxidants such as OH and no-radical oxidants such H_2O_2. Moreover, the model study shows the importance of the aqueous phase for the formation of higher oxidised organic compounds such as substi-

tuted mono- and diacids. In particular, the aqueous phase oxidations of methylglyoxal and 1,4-butenedial have been identified as important OH radical sinks under urban environmental conditions.

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