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SPACCIM simulations of chemical aerosol-cloud interactions with the multiphase chemical mechanism MCM-CAPRAM3.0i

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Heterogeneous and multiphase processes in fog droplets, cloud droplets and deliquescent particles can potentially alter the physico-chemical composition of the tropospheric aerosol on global scale. In order to model such complex tropospheric multiphase chemical interactions of clouds, fogs and deliquescent aerosol particles, chemical mechanisms with a detailed description of chemical processes in both the gas and aqueous phase are required. Currently, both near-explicit gas and aqueous phase mechanisms are available. However, a near-explicit chemical multiphase mechanism was still missing. Therefore, the near-explicit chemical gas phase mechanism MCM v3 (Master Chemical Mechanism, Saunder et al., 2003) with about 13502 reactions and the explicit aqueous phase mechanism CAPRAM3.0i (Chemical Aqueous Phase Radical Mechanism, Herrmann et al., 2005) with about 777 reactions were coupled and integrated into the model framework SPACCIM (SPectral Aerosol Cloud Chemistry Interaction Model; Wolke et al., 2005). The parcel model SPACCIM combines a complex microphysical and multiphase chemistry model.
First SPACCIM simulations have been carried out for different environmental conditions using a non-permanent cloud scenario. The model studies were aimed to investigate multiphase chemistry in tropospheric deliquescent aerosol particles, fogs and clouds in more detail. The model investigations were focused on the multiphase chemistry of tropospheric radical oxidants such as OH and NO3, organic compounds and closely linked chemical subsystems. The model results have been analysed including time-resolved reaction flux analyses. The obtained model results of the near-explicit multiphase mechanism MCM-CAPRAM3.0i have been compared with results of former model studies using the non-explicit gas phase mechanism RACM-MIM2ext and CAPRAM3.0i (Tilgner and Herrmann, 2010).

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