Combining MCM and CAPRAM: First Results and Outlook

H. Herrmann, A. Tilgner, R. Schrödner, P. Bräuer, and R. Wolke
Leibniz-Institut für Troposphärenforschung, Leipzig, Germany (herrmann@tropos.de)

Multiphase chemical processes in the tropospheric clouds and deliquescent particles are expected to proceed very efficient on short timescales and hence they are able to alter the chemical aerosol composition and the deduced physical properties on a global scale. Nevertheless, the chemical multiphase processing, e.g. the secondary chemical formation and aging of organic aerosol constituents, remains poorly considered in current multiphase models. To model complex tropospheric multiphase interactions, chemical mechanisms with a detailed gas and aqueous phase chemistry description are necessary. Both near-explicit gas and aqueous phase mechanisms are presently available. However, a near-explicit chemical multiphase mechanism which includes a detailed organic chemistry in either phase was still missing. Hence, the near-explicit chemical gas phase mechanism MCM v3 (Master Chemical Mechanism, http://mcm.leeds.ac.uk/MCM/) with about 13502 reactions was coupled to the explicit aqueous phase mechanism CAPRAM3.0n (Chemical Aqueous Phase Radical Mechanism, http://projects.tropos.de/capram/) with about 777 reactions and included into the microphysical and multiphase chemistry model framework SPACCIM (SPectral Aerosol Cloud Chemistry Interaction Model).
First model studies were performed for different environmental conditions using a non-permanent cloud scenario to study the tropospheric multiphase chemistry in more detail. The model investigations were focused mainly on multiphase chemistry of tropospheric oxidants and closely linked organic chemical subsystems.
A scoping study focusing on future MCM-CAPRAM coupling revealed that ~60% of the MCM compounds might undergo efficient phase transfer and perhaps aqueous phase chemistry which needs to be integrated in future CAPRAM versions. Accordingly, necessary prospective efforts and needs for the ongoing CAPRAM mechanism development are outlined to derive more detailed description of the aqueous organic chemistry comparable to the MCM chemistry in the future.