CAPRAM2.4: An updated and revised Chemical Aqueous Phase Radical Mechanism describing tropospheric cloud chemistry

A contribution to subproject CMD-MPM

B. Ervens, R. Wolke and H. Herrmann

Institut für Troposphärenforschung, Permoserstr. 15, D-04303 Leipzig, Germany

The actual version of the **C**hemical **A**queous **P**hase **Ra**dical **M**echanism (CAPRAM2.4), describing in detail chemical processes in tropospheric clouds contains 440 aqueous phase processes which are coupled by uptakes (resistance model by Schwartz, 1986) for 34 species to the gas phase mechanism RACM (Stockwell *et al.*, 1997). The results presented show (i) the differences to the former version (version 2.3, Herrmann *et al*., 2000), and (ii) effects which are caused by consideration of emissions and depositions in the box model.

Within the update of the former version of CAPRAM mainly the chemistry of the transition metal ions (TMI: Fe, Mn, Cu), and of the organics was revised and completed: On the one hand species such as FeO^{2+} and $FeCH_3O_2^{2+}$ are included representing oxidation pathways for iron and on the other hand the oxidation of organics is formulated explicitly by alkyl and peroxyl radicals. Furthermore the detailed chemistry of glyoxal, glyoxylic acid and oxalate was added.

Analysis of reaction pathways clarifies that extended TMI chemistry causes an enhanced H_2O_2 production leading to the total oxidation of sulfur(IV) during the first some hours of the simulation. If emissions and depositions are considered the concentration levels of radicals and also of sulfur(IV) are essentially influenced.

Furthermore a reduced form of CAPRAM2.4 was developed with about 180 aqueous phase processes in which the concentration levels of selected species are comparable (± 2%) to the complete mechanism. It becomes evident that organic oxidation is essentially determined by OH; furthermore it can be stated that the chemistry of manganese and the carbonate radical anion CO_3^- can be neglected under the conditions chosen for the simulations.

References

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