



CAPRAM 3.0: A Mechanism with a more Detailed Description of Tropospheric Aqueous Phase Organic Chemistry

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Tropospheric aqueous phase chemical processes which are not only restricted to cloud chemical conversions but also include deliquescent particle chemistry might have profound effects in atmospheric chemistry. Up to now, only few studies have attempted to characterise the conversions of higher organics within the tropospheric aqueous phase and it should be noted that the clear description and documentation of the applied chemical mechanism in full detail is a prerequisite for such modelling studies.

CAPRAM 3.0 is the latest development of CAPRAM (Chemical Aqueous Phase Radical Mechanism) series which is incorporating CAPRAM 2.4 and a new extended reaction mechanism for atmospheric-relevant hydrocarbons containing more than two and up to six carbon atoms. The chemistry of organics containing three and four carbon atoms is now in details described. Almost 400 new reactions are now implemented considering the chemistry of organic compounds containing different functional groups, i.e. alcohols, carbonyl compounds, mono- and dicarboxylic acids, poly-functional compounds as well as some esters and heterocyclic compounds.

The aqueous chemistry has been coupled to the gas phase mechanism RACM (Regional Atmospheric Chemistry Modeling), and phase exchange is treated using the resistance model of Schwartz (1986).

The CAPRAM remote scenario which was chosen as standard scenario showed that the introduction of the higher organic chemistry has relevant influence on the standard subsystems. The diurnal peak concentration of OH radical in the droplets decreases

with about 40% and the reactions of OH with hydrocarbons containing 3 or 4 carbon atoms account for about 10% out of the total sinks of OH in the droplets. A slightly stronger acidification of the aqueous phase in comparison to CAPRAM 2.4 is observed.

The formation and accumulation phase of substituted mono and dicarboxylic acids such as tartaric, mesoxalic and acetic acid in the aqueous is also observed.