4.046 Development of a new explicit oxidation mechanism of organics in clouds.

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Abstract:

Secondary organic aerosol (SOA) may form as a result of chemical reactions in cloud droplets which are referred to as “cloud aqSOA”. Clouds can dissolve organic vapors in the aqueous phase where these compounds are transformed into SOA. Accretion and oxidation processes may compete in the aqueous phase. Cloud chemistry acts both as a source for SOA (through oligomerization and functionalization reactions) and as a sink for SOA (through fragmentation reactions).
Cloud chemistry has been developed to represent and evaluate these chemical processes and recent modeling studies aimed at implementing newly identified accretion processes to evaluate their potential impacts on SOA formation. However, a matching accurate knowledge of aqueous oxidation is required since oxidation processes may control the organic radicals availability to form “accretion” products. Due to the numerous organic compounds found in cloud water, several oxidation pathways are not fully documented. To remedy this lack of information, structure activity relationships (SAR) are now available in the literature for estimating missing parameters such as kinetic constants, branching ratios, hydration constants, acidity constants, *etc.* Based on these structure-activity relationships, a new detailed aqueous phase mechanism (CLEPS: CLoud Explicit Physico-chemical Scheme) describing the oxidation of soluble organic compounds resulting from isoprene oxidation is proposed.
This new aqueous phase mechanism is coupled with the detailed gas phase mechanism MCM v3.3. The GROMHE SAR allows for the evaluation of Henry's law constants for organic compounds. Variable photolysis in both gas and aqueous phases using the TUV 4.5 radiative transfer model is calculated. The resulting multiphase mechanism has been implemented in a cloud chemistry model, using a warm microphysical scheme module. Sensitivity tests experiments are presented on oxygenated compounds produced by the isoprene oxidation.