Geophysical Research Abstracts,
Vol. 11, EGU2009-4805, 2009
EGU General Assembly 2009

Reactivity of polyfunctional alcohols towards atmospheric radicals in the aqueous solution

D. Hoffmann and H. Herrmann

Leibniz-Institut für Troposphärenforschung, Chemistry, Leipzig, Germany (hoffmann@tropos.de)

Alcohols such as ethylene glycol, propylene glycol and glycerol are widely used compounds in numerous applications. The oxidation of these compounds can influence the tropospheric oxidation budget as well as contribute significantly to the formation of low volatile organic particle constituents, such as mono- and dicarboxylic acids. Model simulations applying the multiphase chemistry mechanism CAPRAM 3.0i (Chemical Aqueous Phase Radical Mechanism) show that the aqueous phase oxidation of ethylene glycol contribute significantly to the formation of the known particle constituent oxalic acid under remote (up to 1.7%) and urban (up to 9.5%) conditions. Due to their high solubility oxidation processes of polyalcohols will take place mainly in the aqueous solution. Oxidation reactions of alcohols are triggered by reactions with atmospheric radicals such as OH, NO3 and SO4-. However, for the detailed implementation of the tropospheric degradation of alcohols in atmospheric chemistry mechanisms many kinetic data, in particular as a function of the temperature, are still needed.
Therefore, the reactivity of 1,2-ethanediol (ethylene glycol), 1,2-propanediol (propylene glycol), 1,3-propanediol, 1,2,3-propanetriol (glycerol), 1,2-butanediol, 1,4-butanediol and 1,5-pentanediol was systematically investigated towards OH, NO3 and SO4- radicals in the aqueous solution. All kinetic measurements were done as a function of the temperature. During these experiments the temperature of the measurement solution was varied between $278 \leq T\ [K] \leq 318$. Experiments were carried out using laser flash photolysis technique at a wavelength of 248 nm. Rate constants were measured directly or using competition kinetics in case of OH. The kinetic data and activation parameters obtained will be summarized and discussed with available literature data. Furthermore, the data obtained will be discussed in terms of reactivity correlations and atmospheric relevance. A more detailed implementation of the aqueous phase radical chemistry of alcohols into multiphase reaction mechanisms will contribute to a better understanding of tropospheric particle mass production processes in the troposphere.