Modeling Multiphase Chemical Kinetics of OH Radical Reacting with Biomass Burning Organic Aerosol

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Levoglucosan, abietic acid and nitroguaiacol are commonly used as molecular tracers of biomass burning in source apportionment. Recent studies have demonstrated the decay of levoglucosan when the particles were exposed to atmospherically relevant concentration of OH radicals [1-3]. However, multiphase chemical kinetics of OH radical reacting with such compounds has not fully understood. Here we apply the kinetic multi-layer model for gas-particle interactions (KM-GAP) [4] to experimental data of OH exposure to levoglucosan, abietic acid and nitroguaiacol [1]. KM-GAP resolves the following mass transport and chemical reactions explicitly: gas-phase diffusion, reversible surface adsorption, surface reaction, surface-bulk transport, bulk diffusion and reaction. The particle shrink due to the evaporation of volatile reaction products is also considered. The time- and concentration-dependence of reactive uptake coefficient of OH radicals were simulated by KM-GAP. The measured OH uptake coefficients were fitted by a Monte Carlo (MC) filtering coupled with a genetic algorithm (GA) to derive physicochemical parameters such as bulk diffusion coefficient, Henry's law coefficient and desorption lifetime of OH radicals. We assessed the relative contribution of surface and bulk reactions to the overall uptake of OH radicals. Chemical half-life and the evaporation time scale of these compounds are estimated in different scenarios (dry, humid and cloud processing conditions) and at different OH concentrations.

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