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Kinetic model framework for aerosol and cloud surface chemistry and gas-particle interactions: exemplary numerical simulations for steady-state systems

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A kinetic model framework with consistent and unambiguous terminology and universally applicable rate equations and parameters for aerosol and cloud surface chemistry and gas-particle interactions is presented in companion papers by Pöschl, Rudich, and Ammann (2005a,b), abbreviated PRA. It allows to describe mass transport and chemical reaction at the gas-particle interface and to link aerosol and cloud surface processes with gas phase and particle bulk processes.

Here we present multiple exemplary steady-state model systems and calculations illustrating how the general mass balance and rate equations of the PRA framework can be easily reduced to compact sets of equations which enable a mechanistic description concentration dependencies of trace gas uptake and particle composition in systems with one or more chemical components and physicochemical processes. The model scenarios illustrate characteristic effects of gas phase composition and basic kinetic parameters on the rates of mass transport and chemical reactions. They demonstrate how adsorption and surface saturation effects can explain non-linear gas phase concentration dependencies of surface and bulk accommodation coefficients, uptake coefficients, and bulk solubilities (deviations from Henry's law). Such effects are expected to play an important role in many real atmospheric aerosol and cloud systems involving a wide range of organic and inorganic components of concentrated aqueous and organic solution droplets, ice crystals, and other crystalline or amorphous solid particles (Ammann and Pöschl, 2005a). Numerical simulations of time-dependent systems are presented in a companion paper (Ammann and Pöschl, 2005b).

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References

Ammann, M. and Pöschl, U.: Kinetic model framework for aerosol and cloud surface chemistry and gas-particle interactions: Part 2 - exemplary practical applications and numerical simulations, Atmos. Chem. Phys., submitted, 2005a.

Ammann, M. and Pöschl, U.: Kinetic model framework for aerosol and cloud surface chemistry and gas-particle interactions: exemplary numerical simulations for time-dependent systems, EGU General Assembly 2005, Vienna, 2005b.

Pöschl, U., Rudich, Y., and Ammann, M.: Kinetic model framework for aerosol and cloud surface chemistry and gas-particle interactions: Part 1 - general equations, parameters, and terminology, Atmos. Chem. Phys., submitted, 2005a.

Pöschl, U., Rudich, Y., and Ammann, M.: Kinetic model framework for aerosol and cloud surface chemistry and gas-particle interactions, EGU General Assembly 2005, Vienna, 2005b.