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

M. Ammann (1) and U. Pöschl (2)

(1) Paul Scherrer Institute, Switzerland (2) Technical University of Munich, Germany (markus.ammann@psi.ch)

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 time-dependent 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 of time and concentration dependencies of trace gas uptake and particle composition in systems with one or more chemical components and physicochemical processes. The model scenarios show the effects of reversible adsorption, surface-bulk transport, and chemical aging on the temporal evolution of trace gas uptake by solid particles and solubility saturation of liquid particles. They demonstrate how the transformation of particles and the variation of trace gas accommodation and uptake coefficients by orders of magnitude over time scales of microseconds to days can be explained and predicted from the initial composition and basic kinetic parameters of model systems by iterative calculations using standard spreadsheet programs. Moreover, they show how apparently inconsistent experimental data sets obtained with different techniques and on different time scales can be efficiently linked and mechanistically explained by application of consistent model formalisms and terminologies within the PRA framework (Ammann and Pöschl, 2005a). Numerical simulations

of steady-state systems are presented in a companion paper (Ammann and Pöschl, 2005b).

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