Development of a kinetic model framework and master mechanism of aerosol surface chemistry and gas-particle interactions

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Keywords: Aerosol modeling, aerosol-surface interactions, aerosol-surface reactions

Atmospheric aerosols are ubiquitous in the atmosphere. They have the ability to impact cloud properties, radiative balance and provide surfaces for heterogeneous reactions. The uptake of gaseous species on aerosol surfaces impacts both the aerosol particles and the atmospheric budget of trace gases. These subsequent changes to the aerosol can in turn impact the aerosol chemical and physical properties. However, this uptake, as well as the impact on the aerosol, is not fully understood. This uncertainty is due not only to limited measurement data, but also a dearth of comprehensive and applicable modeling formalizations used for the analysis, interpretation and description of these heterogeneous processes. Without a common model framework, comparing and extrapolating experimental data is difficult. In this study, a novel kinetic model framework was developed to describe the uptake and interactions of gas phase species and particles (Ammann & Pöschl, 2005; Pöschl et al., 2005).

Figure 1: Representation of resolution of particle and gas layers in the model.

The processes occurring at each layer can be fully described using known fluxes and kinetic parameters. Using this system there is a clear separation of gas phase, gas-surface and surface bulk transport and reactions. The compound described in Figure 1, compound “Z_k”, is semi-volatile and thus found in all layers. Its partitioning can be calculated using the various flux values (J) shown in Figure 1. By describing these layers unambiguously and precisely, the interactions of all species in the system can be appropriately modeled.

Using this framework, various systems have been modeled. Results of the uptake of various gas phase species into both liquid and solid particles will be discussed.

This work was supported by the European Integrated project on Aerosol Cloud Climate and Air Quality Interactions (EUCARRI).
