



## **Modeling aerosol chemistry and gas-particle interactions with the kinetic double-layer surface model K2-SURF: Oxidation of polycyclic aromatic hydrocarbons (PAHs)**

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Aerosol particles are ubiquitous in the atmosphere. They have the ability to impact cloud properties, the Earth's radiative balance and provide surfaces for heterogeneous reactions. The uptake of gaseous species on aerosol surfaces impacts both the particle properties and the atmospheric budget of trace gases. 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 framework, comparing and extrapolating experimental data is difficult. In this study, a novel kinetic double layer surface model (K2-SURF) has been developed and applied to describe the oxidation of a variety of polycyclic aromatic hydrocarbons (PAHs).

K2-SURF is based on the kinetic model framework for aerosol and cloud surface chemistry and gas particle interactions proposed by Pöschl, Rudich and Ammann (PRA, Ammann and Pöschl 2007; Pöschl et al. 2007). It shall serve as a basis for the development of a detailed master mechanism, simplified mechanism and parameterizations of atmospheric aerosol chemistry analogous to existing mechanisms and parameterizations of atmospheric gas-phase chemistry.

One of the key aspects is the defining of clear distinctions between various lay-

ers/compartments of the particle and surrounding gas phase (gas phase, near-surface gas phase, sorption layer, quasi-static surface layer, near-surface bulk and bulk). 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. By describing these layers unambiguously and precisely, the interactions of all species in the system can be appropriately modeled. However, such detail is not necessary for all systems and the model can easily be simplified.

In describing the oxidation of polycyclic aromatic hydrocarbons (PAHs), the focus is on the interactions between the sorption layer and quasi-static surface layer. The results from a variety of published experimental studies were analyzed and compared utilizing K2-SURF. These comparisons as well as the atmospheric implications will be presented.

## REFERENCES

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