EGU21-9292
https://doi.org/10.5194/egusphere-egu21-9292
EGU General Assembly 2021

The impact of non-ideality on reconstructing spatial and temporal variations of aerosol acidity with multiphase buffer theory

Yafang Cheng[1], Guangjie Zheng[1], Hang Su[2], Siwen Wang[2], and Andrea Pozzer[3]
[1]Minerva Research Group, Max Planck Institute for Chemistry, Mainz 55128, Germany
[2]Multiphase Chemistry Department, Max Planck Institute for Chemistry, Mainz 55128, Germany
[3]Air Chemistry Department, Max Planck Institute for Chemistry, Mainz 55128, Germany

Aerosol acidity is a key parameter in atmospheric aqueous chemistry and strongly influence the interactions of air pollutants and ecosystem. The recently proposed multiphase buffer theory provides a framework to reconstruct long-term trends and spatial variations of aerosol pH based on the effective acid dissociation constant of ammonia ($K_{a,NH3}^*$). However, non-ideality in aerosol droplets is a major challenge limiting its broad applications. Here, we introduced a non-ideality correction factor (c_{ni}) and investigated its governing factors. We found that besides relative humidity (RH) and temperature, c_{ni} is mainly determined by the molar fraction of NO_3^- in aqueous-phase anions, due to different NH_4^+ activity coefficients between $(NH_4)_2SO_4$- and NH_4NO_3-dominated aerosols. A parameterization method is thus proposed to estimate c_{ni} at given RH, temperature and NO_3^- fraction, and is validated against long-term observations and global simulations. In the ammonia-buffered regime, with c_{ni} correction the buffer theory can well reproduce the $K_{a,NH3}^*$ predicted by comprehensive thermodynamic models, with root-mean-square deviation ~0.1 and correlation coefficient ~1. Note that, while c_{ni} is needed to predict $K_{a,NH3}^*$ levels, it is usually not the dominant contributor to its variations, as ~90% of the temporal or spatial variations in $K_{a,NH3}^*$ is due to variations in aerosol water and temperature.