

Leipziger Meteorologisches Kolloquium

Donnerstag, 26.01.2023, 14.00 Uhr, TROPOS, Seminarraum, Geb. 23.1 und online

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Oxidants in the atmospheric multiphase system - new insights and their implications

Box models are commonly used to simulate the cycling of reactive oxygen species (ROS, e.g., OH, HO₂ and H₂O₂), and their oxidation rates of organic and inorganic species within the atmospheric multiphase (gas + aqueous) system. In such models, simplified assumptions are often made regarding basic microphysical and physico-chemical droplet properties, such as cloud droplet size and homogeneity of chemical composition. In addition, the presence of biological cloud water constituents and their role in degrading organics is ignored.

In my talk, I will give an overview of the extent to which such assumptions affect predictions of ROS levels and their reactions. Specifically, I will focus on three aspects:

(i) The phase transfer rates of ROS and related compounds are a function of the cloud droplet size. Therefore, differences in oxidation rates are predicted depending on the cloud droplet size (distribution).

(ii) The significant role of transition metal ions (iron, copper) for redox cycling of ROS has been highlighted. In many previous model studies. Transition metals have distinct emission sources, which implies that they are only present in a subset of particles, and, thus, cloud droplets. This fact has not been considered in model studies so far. I will demonstrate how more realistic assumptions on iron (copper) distributions affect ROS redox cycling and metal oxidation states.

(iii) Even though only a small subset of cloud droplets contains metabolically active bacteria cells, I will show under which conditions biodegradation is predicted to be a potentially significant loss of small carboxylic acids, in addition to their oxidation by OH. It will be discussed how and for which compounds biodegradation processes should be added to atmospheric multiphase chemistry models.

In summary, my talk will provide an overview on the needs to extend traditional atmospheric multiphase chemistry models, as well as on the measurements that are required to further constrain such models.