

Numerical modeling of sulfur and ammonium chemistry in the clouds

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To understand how clouds affect chemical constituents and their distributions, numerical modeling the chemistry in clouds has been an active area of research. In recent years there has been considerable interest in the roles that clouds and precipitation play in cycles of various tropospheric chemical species, especially sulfur and nitrogen. This is very complex problem. Many processes must be taken into account to describe the effects of clouds on tropospheric chemistry, including cloud dynamics, microphysics and chemistry.

In this paper, an aqueous chemistry model was incorporated into 3D cloud-resolving mesoscale ARPS (Advanced Regional Prediction System) model developed in the Center for analysis and prediction of storms (CAPS) at the University of Oklahoma. The general method for parametrize chemical processes in the model is similar to that described by Taylor (1989). The absorption of a gas phase chemical species in the cloud water and rainwater is calculated either by the equilibrium according to Henry's law and by more accurate real kinetic calculation of gas uptake. Six water categories was considered: water vapor, cloud water, rainwater, cloud ice, hail and snow. Each chemical constituent in each microphysical category was represented by differential equation for mass continuity. The source and sink terms in equations of continuity represent either transfer of a chemical species from one microphysical category to another (e. g. transfer of cloud ice sulphate to cloud water sulfate by melting, transfer of cloud water sulfate to rainwater sulfate by autoconversion etc.) or a chemical reaction (e. g. oxidation of cloud water SO₂ by H₂O₂ and O₃ to cloud water sulfate). Comprised microphysical processes in source/sink terms are: autoconversion, accretion, Bergeron processes, freezing, depositional growth, melting, sublimation and evaporation. The calculation of the cloud water pH and rainwater pH was based on the equilibrium hydrogen ion concentration ($\text{pH} = -\log[\text{H}^+]$) with an assumption that HSO₃⁻ is the dominant form of aqueous S(IV) in cloud water and precipitation.