Model Evaluations of Heterogeneous Nitryl Chloride Production

Speakers

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Nitryl chloride (ClNO2) is an important nighttime precursor to reactive chlorine radicals in the troposphere. Recent ambient observations showed high correlations of ClNO2 and N2O5 mixing ratios, suggesting that the main production pathway of ClNO2 in the polluted atmosphere is through N2O5 heterogeneous hydrolysis on chloride-containing aerosols. Thus in the presence of particulate chloride, N2O5 heterogeneous hydrolysis can no longer be considered a removal pathway for NOx, as ClNO2 is a reservoir species that can release NO2 during the daytime through photolysis. Consequently, ClNO2 has high potentials for altering the oxidative capacity of the atmosphere. There are many challenges with quantifying the impact of ClNO2 through models, including the parameterization of the N2O5 heterogeneous reaction process, which is dependent on meteorological conditions and aerosol compositions, the ClNO2 production yields, and uncertainties with sources of particulate chloride. Using the WRF-Chem as the host model, we tested several state-of-the-art N2O5 heterogeneous hydrolysis parameterizations, taking into account the uptake enhancement by the presence of particulate chloride, and the uptake suppression by nitrate and organic coatings. The model results are evaluated against observations made during the CalNex 2010 measurement campaign. We will present the model performance in simulating ClNO2 by the various parameterization methods, and show the sensitivity of ClNO2 production to spatial and temporal variations in anthropogenic chlorine emission sources, as well as the resulting impact on criteria pollutants in the South Coast Air Basin of California.