

Model Evaluations of Heterogeneous Nitryl Chloride Production

Speakers

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Nitryl chloride (CINO₂) is an important nighttime precursor to reactive chlorine radicals in the troposphere. Recent ambient observations showed high correlations of CINO₂ and N₂O₅ mixing ratios, suggesting that the main production pathway of CINO₂ 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 NO_x, as CINO₂ is a reservoir species that can release NO₂ during the daytime through photolysis. Consequently, CINO₂ has high potentials for altering the oxidative capacity of the atmosphere. There are many challenges with quantifying the impact of CINO₂ through models, including the parameterization of the N₂O₅ heterogeneous reaction process, which is dependent on meteorological conditions and aerosol compositions, the CINO₂ 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 CINO₂ by the various parameterization methods, and show the sensitivity of CINO₂ 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.

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