Geophysical Research Abstracts
Vol. 21, EGU2019-12444, 2019
EGU General Assembly 2019

Modeling the impact of heterogeneous reactions of chlorine on summertime nitrate formation in Beijing, China

Xionghui Qiu
Qinghua University, School of Environment, China (qiuxh1986@163.com)

A comprehensive chlorine heterogeneous chemistry is incorporated into the Community Multiscale Air Quality (CMAQ) model to evaluate the impact of chlorine-related heterogeneous reaction on diurnal and nocturnal nitrate formation and quantify the nitrate formation from gas-to-particle partitioning of HNO_3 and from different heterogeneous pathways. The results show that these heterogeneous reactions increase the atmospheric Cl2 and $ClNO_2$ level, leading to an increase of the nitrate concentration by $\sim$10% in the daytime. However, these reactions also lead to a decrease the nocturnal nitrate by $\sim$20%. Sensitivity analyses of uptake coefficients show that the empirical uptake coefficient for the O_3 heterogeneous reaction with chlorinated particles may lead to the large uncertainties in the predicted Cl2 and nitrate concentrations. The N2O5 uptake coefficient with particulate Cl- concentration dependence performs better to capture the concentration of $ClNO_2$ and nocturnal nitrate concentration. The reaction rate of OH and NO_2 in daytime increases by $\sim$15% when the heterogeneous chlorine chemistry is incorporated, resulting more nitrate formation from HNO_3 gas-to-particle partitioning. By contrast, the contribution of the heterogeneous reaction of N2O5 to nitrate concentrations decreases by about 27% in the nighttime when its reactions with chloriated particles are considered. However, the generated gas-phase $ClNO_2$ from the heterogeneous reaction of N2O5 and chlorine-containing particles further decompose to increase the nitrate by 6%. In general, this study highlights the potential of significant underestimation of daytime and overestimation of nighttime nitrate concentrations for chemical transport models without proper chlorine chemistry in the gas and particle phases.