The Importance of Heterogeneous Reaction of NOx and NOy in the Regional Chemical Transport Models for Ozone Simulation

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The regional models for simulating ozone pollution have been developed substantially in the last couple of decades, and are now in general thought to reproduce the observational data reasonably well. However, the recent model-intercomparison study in East Asia, MICS-Asia III project, has revealed this is not necessarily true and relatively large discrepancy among models and between model simulation and observational data have been revealed. The purpose of this study is to elucidate the cause of the discrepancies and to propose the revision of regional model simulation for ozone pollution. So far, model simulation of ozone pollution has been conducted mostly tageting only for O_3 and much of efforts have not been made for the reproduction of observational data of key precursors, NO_x and VOCs. However, when the model simulation will be used for policy tools in such a way as the future prediction of O3 concentration responding to the emission control of NO_x and VOCs, the reproduction of the present concentrations of NO_x and VOC are thought to be important in order to improve the reliability of the modelsimulation.

For example, as for NO_x the following problems have been pointed out by the comparison between the urban field observation and model simulation.

- 1. In the uraban atmosphere, ${\rm HNO_3}$ concentrations are overestimated and ${\rm NO_2}$ concentrations are underestimated.
- 2. In the urban atmosphere high concentrations of HONO are observed even in daytime and the formation processes have not been quantified
- 3. Under high NO_x conditions, OH/HO₂ concentrations are underestimated.

In the present study, the cause of these phenomena are ascribed to the following heterogeneous reactions of NO_x and NO_y on aerosol surfaces,

HNO₃ + aerosol ---> NO₂

NO₂ + aerosol ---> HONO

and discussion will be made.

Further, the results of process analysis of vertical and horizontal transport, net chemical production and deposition loss of O_3 among models will be made for the simulation results of MICS-Asia III in Beijing and Tokyo.

Keywords: ozone, NOx, NOy, heterogeneous reactions, regional chemical transport model