Geophysical Research Abstracts
Vol. 19, EGU2017-11029-3, 2017
EGU General Assembly 2017

Impacts of heterogeneous chemistry on heavy pollution in the JJJ (Beijing-Tianjin-Hebei) region

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The NO_2 heterogeneous reaction on soot surfaces was incorporated into the WRF-Chem model to assess the impacts of the heterogeneous chemistry on the concentrations of HONO, HO_x, O_3, NO_3-, and NH4+ in the JJJ (Beijing-Tianjin-Hebei) region. Results showed that the soot redox process with a γ value of 10-4 at night and the soot heterogeneous photochemistry with the γ formula of JNO_2/10 in the daytime yielded a nighttime HONO increase of 0.4–1.8 ppb and a percentage enhancement of 10%–50% for HO_x, 2%–6% for O_3, 5%–21% for NO_3-, and 6%–17% for NH4+ in the major cities of the JJJ region. The HONO simulations in this case were reasonable compared with observations in Beijing. Minor enhancements were found for HONO, HO_x, O_3, NO_3-, and NH4+, with a maximum increase of $\sim$0.2 ppb for HONO and $\leq$ $\sim$6% for HO_x, O_3, NO_3-, and NH4+ when γ was $\leq$ 10-5. When γ was increased to 10-3, produced are a nighttime maximum enhancement of $\sim$8.6 ppb for HONO, and a maximum percentage enhancement of $\sim$79% for HO_x, $\sim$17% for O_3, $\sim$211% for NO_3-, and $\sim$152% for NH4+. This case considerably overestimated HONO and NO_3- concentrations in Beijing in most cases. The soot surface area per unit volume of air (As) was another key parameter for the NO_2 heterogeneous reaction on soot. The As values showed a sharp decrease from 3$\times$103 μm2 cm-3 near the ground to 6$\times$102 μm2 cm-3 at $\sim$200 m at night. Although the surface areas of major aerosol components at nighttime were [U+F07E] three times larger than that of those in the daytime, the surface area fractions of the major aerosol components showed minor variations between day and night. The surface area fractions of NO_3-, SO42-, and soot were 32%–36%, 25%–28%, and 25%–26%, respectively.