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Heterogeneous chemistry: a mechanism missing in current models to explain secondary inorganic aerosol formation during the January 2013 haze episode in North China

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The Data for Model Performance Evaluation

National Climate Data Center (NCDC) contains measurement data of major meteorological parameters such as wind and temperature every 1 or 3 h. These data can be accessible via ftp://ftp.ncdc.noaa.gov/pub/data/noaa/. To evaluate the meteorological fields produced by Weather Research and Forecasting (WRF), five meteorological variables that influence the accuracy of air quality modeling are selected: temperature at 2 m (T2), RH at 2 m (RH2), wind speed at 10 m (WS10), wind direction at 10 m (WD10), and daily mean precipitation (Precip), as in previous studies (Zhang et al., 2006, 2011; Wang et al., 2010; Liu et al., 2010). T2 and RH2 are selected for evaluation because they have significant effects on rate constants of atmospheric chemistry. The accuracy of the modeled WS10 and WD10 are very important because the horizontal transport of pollutants is sensitive to wind and overestimated WS10 can cause underestimates in the concentrations of air pollutants in the source regions (Liu et al., 2010). The Precip is evaluated because it is the driving force for wet deposition of air pollutants and the precipitating clouds can enhance SO_4^{2-} formation via the aqueous-phase chemistry.

China National Environmental Monitoring Center (CNEMC) published hourly concentrations of SO_2, NO_2, CO, O_3, $PM_{2.5}$, and PM_{10} from 496 national monitoring stations located in 74 major cities (about 20% of the total cities in China) since January 2013. The number of cities reporting these data has increased to 190 since January 2014. These data can be accessible via http://113.108.142.147:20035/emcpublish/. The O_3 data in the January 2013 has some mistakes because the values in one day are always the same. In this study, all the pollutants except O_3 are used to evaluate the CMAQ performance.

Tsinghua University site (THU) dataset contains hourly concentrations of major particulate species (SO_4^{2-}, NO_3^-, NH_4^+, EC, and OC) measured during January 2013. The site (40°0′17″ N, 116°19′ 34″ E) is located in the campus of Tsinghua University, northwest of urban Beijing. The $PM_{2.5}$ is measured by the PM-712 Monitor (Kimoto Electric Co., Ltd., 2012). Sulfate and nitrate in $PM_{2.5}$ are measured using ACSA-08 Monitor (Kimoto et al., 2013). Ammonium is predicted on the basis of sulfate and nitrate concentrations. EC and OC are measured using the Sunset Model 4 semi-continuous OC/EC analyzer (Beaverton, Oregon, USA) with the NIOSH (National Institute for Occupational Safety and Health) temperature protocol.

Table S1. Sensitivity simulations of uptake coefficients in R24 with revised CMAQ.

Run Index	Emissions	Meteorology	Model configuration	Purpose
S1	Jan 2013	Jan 2013	revised CMAQ with heterogeneous chemistry, γ_{low}=1E-4 and γ_{high}=2.6E-4 for R24	Evaluate the sensitivity of uptake coefficient in R24 to SNA predictions.
S2	Jan 2013	Jan 2013	revised CMAQ with heterogeneous chemistry, γ_{low}=5E-5 and γ_{high}=1E-4 for R24	
S3	Jan 2013	Jan 2013	revised CMAQ with heterogeneous chemistry, γ_{low}=2E-5 and γ_{high}=5E-5 for R24	
S4	Jan 2013	Jan 2013	revised CMAQ with heterogeneous chemistry, γ_{low}= 1E-5 and γ_{high}= 2E-5 for R24	

Table S2. Uptake coefficients of heterogeneous chemistry used in Revised CMAQ. [a]

Reaction #.	Uptake coefficients (γ_{low})	Uptake coefficients (γ_{high})
R16	1E-4	1E-4
R17	0.1	0.1
R18	0.1	0.1
R19	1E-3	0.1
R20	4.4E-5	2E-4
R21	0.1	0.23
R22	5E-5	5E-5
R23	0.1	0.1
R24	2E-5	5E-5

[a] All uptake coefficients except that of R24 are determined on the basis of Wang et al. (2012).

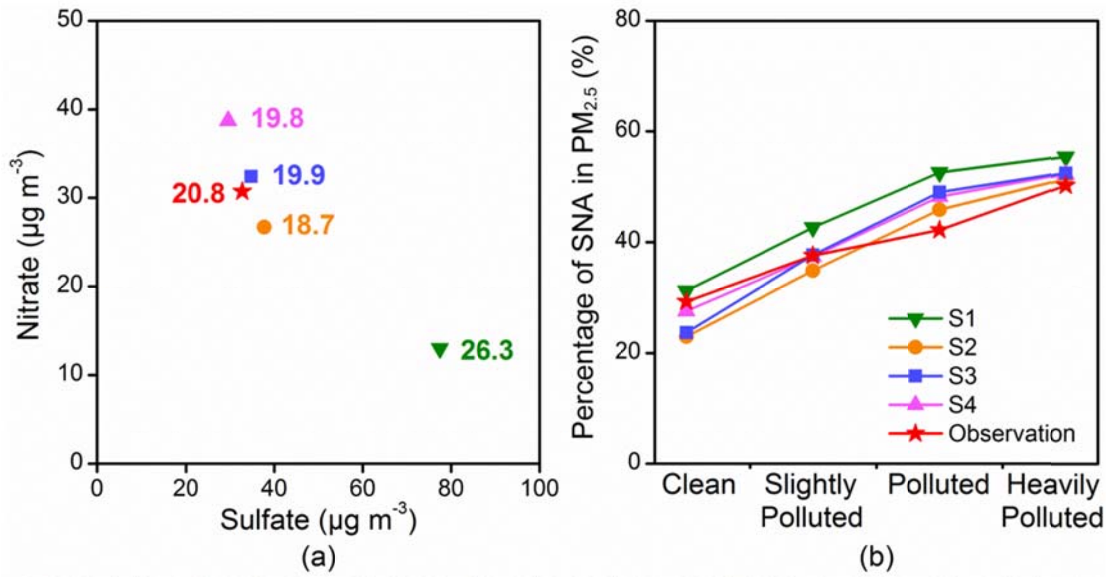

Figure S1. Simulation results of S1, S2, S3 and S4 at the THU site, including (a) concentrations of sulfate, nitrate and ammonium (the number adjacent to each point) and (b) percentages of SNA in the total $PM_{2.5}$.

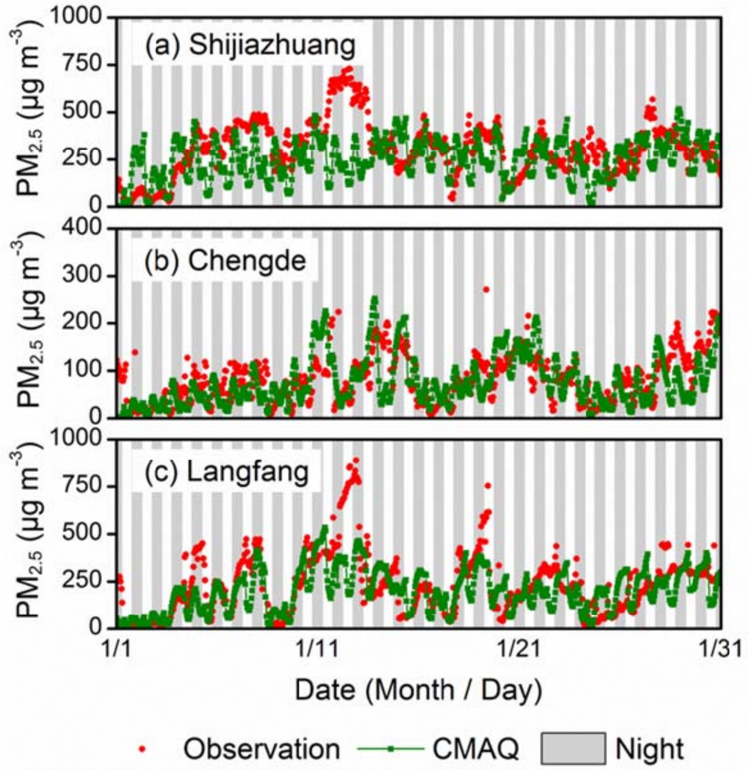

Figure S2. Observed and simulated $PM_{2.5}$ at (a) Shijiazhuang, (b) Chengde and (c) Langfang.

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