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Heterogeneous N_2O_5 reactions on atmospheric aerosols at four Chinese sites: improving model representation of uptake parameters

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S1. Direct measurement of γ_{N2O5} in polluted environments

S1.1 Heshan site

The measurement site was located on a hill (22.73° N, 112.93° E, 60 m a.s.l – above sea level), which was a semi-rural site, southwest of Heshan city in Guangdong Province (Yun et al., 2017). The site was located in the western Pearl River Delta (PRD) with lower economic activity and population density than the central PRD. Three cities of Guangzhou, Foshan and Jiangmen are located 80 km southwest, 50 km southwest and 30 km northeast of the site, respectively. The hill is covered by subtropical trees with limited residents at the foot of the hill and two highways within 3 km.

S1.2 Mount Tai site

The two measurement sites were located on the top of Mount Tai (36.25° N, 117.10° E, 1465 m a.s.l.) in Shandong Province, China (Wang et al., 2017), and the measurement site in 2018 was 400 m southeast of the 2014 site. Two cities of Tai'an and Jinan (the capital of Shandong Province) are located 15 km south and 60 km north of the measurement sites, respectively. The sites are mostly affected by aged air masses and occasionally by plumes from nearby fossil fuel combustion or biomass burning. In 2014, the field campaign was conducted from 24 July to 27 August.

S1.3 Wangdu site

The measurement site was a semi-rural site (38.66° N, 115.20° E) in Wangdu county of Hebei province (Tham et al., 2016). Three cities of Beijing, Tianjin and Shijiazhuang (the capital of Hebei Province) are located 170 km northeast, 180 km east and 90 km southwest of the site, respectively. The site was surrounded by agricultural lands with two highways about 1-2 km away from it and tens of thermal power stations within 200 km. The field campaign was conducted from 21 June to 9 July 2014.

S1.4 Mount Tai Mo Shan site

The measurement site was on the top of Mt. Tai Mo Shan (TMS, 22.41° N, 114.12° E; 957 m a.s.l.) in Hong Kong (Wang et al., 2016). TMS is located in the southeastern PRD region and to the south of Guangdong Province. The measurement site is affected by regional air masses with limited vehicles in the TMS natural reserve. The field campaign was conducted from 15 November to 6 December 2013.

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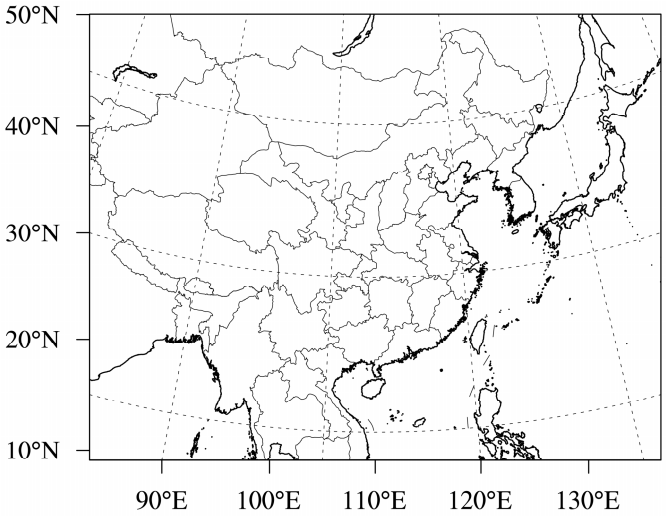

Figure S1. The model domain used in WRF-CMAQ simulation of NO_2 and NO_3^- concentrations.

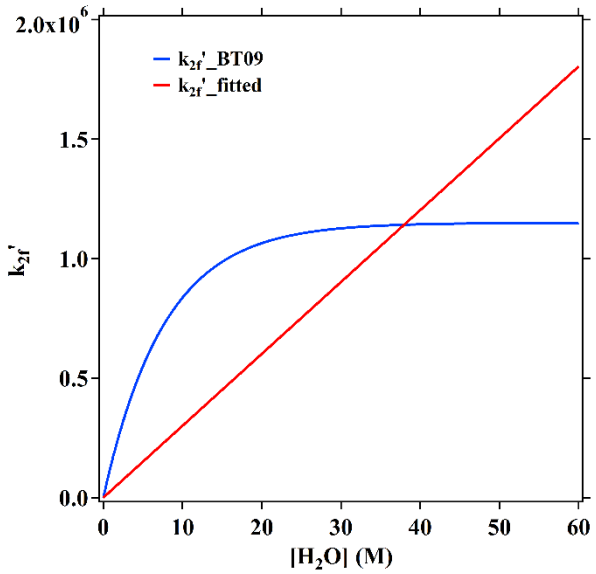

Figure S2. Dependence of the k'_2 derived from the parameterization of BT09 (blue line) and the newly fitted parameterization (red line) on the aerosol H_2O molarity.

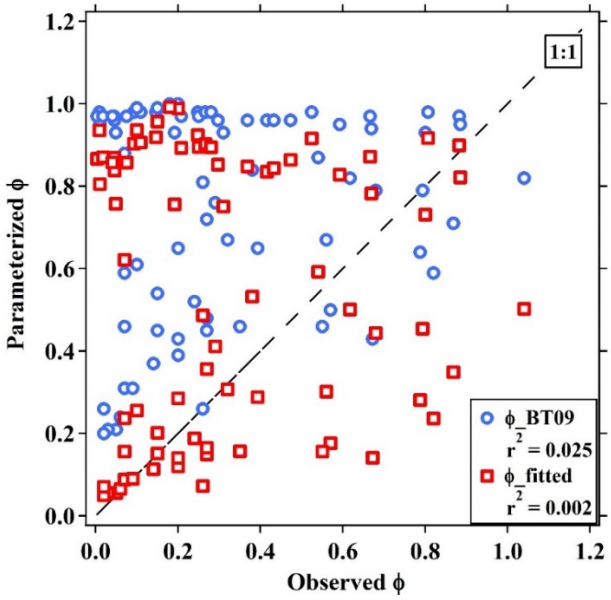

Figure S3. Comparison of the observed Φ_{ClNO2} with the predictions of parameterizations. The dashed line represents the 1:1 line. Blue circles and red squares are results predicted by BT09 parameterization and the observation-based empirical parameterization, respectively.

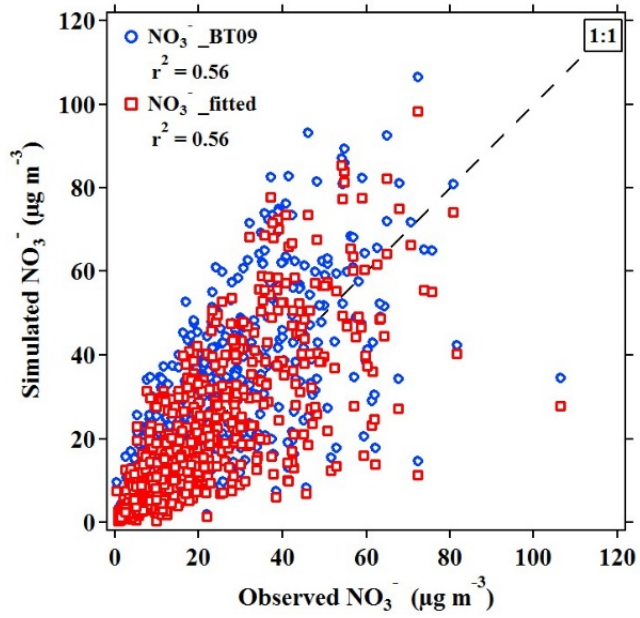

Figure S4. Comparison of the hourly nitrate concentrations from observation and WRF-CMAQ simulation at 29 monitoring sites in North China during December of 2017. The dashed line represents the 1:1 line. Blue circles and red squares are simulation results using BT09 parameterization and the derived observation-based empirical parameterization, respectively.

Table S1. Instruments used for measurement of trace gases and aerosols in Heshan and Mt Tai campaigns.

Species	Measurement technique	Uncertainty	Detection limit	Time resolution
$ClNO_2$, N_2O_5	CIMS	± 25 %	6 pptv	1 min
O_3	UV photometry	± 5 %	0.5 ppbv	1 min
NO	Chemiluminescence	± 20 %	0.06 ppbv	1 min
NO_2	Photolytic converter and chemiluminescence	± 20 %	0.3 ppbv	1 min
Ionic ions of $PM_{2.5}$	GAC-IC	± 10 %	0.01-0.16 μg m^{-3}	30 min
	MARGA	± 25 %	0.001-0.009 μg m^{-3}	60 min
Particle size distribution	SMPS	Particle size range 16.5 - 1000 nm		5 min
	WPS	Particle size range 5 nm - 10 μm		5 min

Table S2. Statistical summary of the averaged observed N_2O_5 uptake coefficients γ_{N2O5}, meteorological and chemical characteristics during the study periods.

Parameter or species	Heshan	Mount Tai
Observed γ_{N2O5}	0.020±0.019	0.011±0.005
T (℃)	22.2±2.2	6.4±5.8
RH (%)	65.5±19.1	61.4±25.4
NO_x (ppbv)	14.0±11.5	2.2±2.1
O_3 (ppbv)	43±22	63±14
NO_x/NO_y	0.59±0.26	0.25±0.19
S_a (um^2 cm^{-3})	1485±910	836±299
$PM_{2.5}$ (μg m^{-3})	66.7±41.9	33.7±26.7
NO_3^- (μg m^{-3})	10.64±11.7	6.67±5.40
Cl^- (μg m^{-3})	1.68±1.63	0.77±0.45