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

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Table S1 Emissions of conventional chemical species in Beijing in 2017 (Unit: ton/a)

Sector	SO_2	NO_X	$PM_{2.5}$	PM_{10}	VOCs	NH_3
Power Plant	842	6267	675	823	70	0
Industry	7421	19867	4545	7059	222046	0
Domestic	12121	10472	14614	19424	53938	8076
Transportation	2365	92024	5080	5255	69908	2475
Agriculture	-	-	-	-	-	18812

Table S2 Comparison of simulated episode average hourly NO_2 and $PM_{2.5}$ and O_3 concentrations with observations averaged from 11 to 15 June 2017 (Obs.: observation, Sim.: simulation). Units: μg m^{-3}

	NO_2				O_3					$PM_{2.5}$			
Sites	Obs	Sim	NMB	NME	Obs	Sim	Sim*	NMB	NME	Obs	Sim	NMB	NME
WSXG	49	54	11%	55%	99	122	121.6	23%	63%	40	38	-6%	53%
DL	21	17	-20%	68%	111	108	107.5	-2%	41%	32	29	-10%	52%
DS	47	53	13%	54%	100	114	113.8	15%	56%	44	41	-7%	53%
TT	40	48	20%	64%	98	130	129.4	33%	60%	37	37	1%	58%
NZG	51	66	28%	62%	111	121	120.5	9%	57%	42	39	-7%	52%
GY	55	65	17%	57%	107	116	115.4	9%	75%	36	33	-8%	54%
WL	52	41	-21%	54%	92	112	111.6	22%	73%	35	33	-7%	54%
XC	43	31	-28%	47%	100	108	107.3	8%	52%	33	29	-12%	55%
HR	26	11	-56%	70%	124	105	104.4	-15%	47%	27	22	-19%	51%
CP	42	28	-34%	58%	96	91	90.3	-5%	77%	33	32	-1%	54%
ATZX	56	62	10%	55%	105	107	106.2	1%	68%	33	31	-4%	54%
GC	56	42	-25%	58%	106	107	106.4	0%	59%	43	37	-14%	52%

WSXG: Wanshouxigong; DL: Dingling; DS: Dongsi; TT:Tiantan; NZG:Nongzhanguan; GY: Guanyuan; WL: Wanliu; XC:Xincheng; HR:Huairou; CP:Changping; ATZX:Aotizhongxin; GC:Gucheng

Sim*: O_3 concentration if the uptake coefficient is increased by a factor of 10

Table 3 The newly added and improved heterogeneous reactions and their uptake coefficients.

Reactions	Uptake Coefficient
$N_2O_5(g) + H_2O(aq) + Cl^-(aq) \rightarrow ClNO_2 + NO_3^-(aq)$	$\gamma_{N_2O_5} = \begin{cases} 0.02, & for\ frozen\ aerosols \\ \frac{4}{v}\frac{V}{S}K_hK_f\left(1 - \frac{1}{\left(\frac{K_3[\mathrm{H_2O}]}{K_2[\mathrm{NO_3^-}]}\right) + 1 + \left(\frac{K_4[\mathrm{Cl^-}]}{K_2[\mathrm{NO_3^-}]}\right)}\right) \end{cases}$
$2NO_2(g) + Cl^-(aq) \rightarrow ClNO(g) + NO_3^-(aq)$	1×10^{-4}
$NO_3 + 2Cl^-(aq) \rightarrow Cl_2(g) + NO_3^-(aq)$	3×10^{-3}
$2Cl^-(aq) + O_3(g) + H_2O(aq) \rightarrow Cl_2(g) + 2OH^-(aq) + O_2(g)$	10^{-3} in the daytime and 10^{-5} in the nighttime
OH(g) + Cl-(aq) →Cl2(g) + 2OH- (aq)	$\gamma = \min(0.04 \times \frac{[Cl^-]}{1000 \times M}, 1)$
$ClONO_2(g) + Cl^-(aq) + H^+(aq) \rightarrow Cl_2(g) + HNO_3(g)$	0.16
$HOCl(g) + Cl^-(aq) + H^+(aq) \rightarrow Cl_2(g) + H_2O(aq)$	1.09×10^{-3}
$ClNO_2(g) + Cl^-(aq) + H^+(aq) \rightarrow Cl_2(g) + HONO(aq)$ (PH < 2.0)	2.65×10^{-6}
$ClNO_2(g) \rightarrow Cl^- + NO_3^- + 2H^+$ (pH ≥ 2.0)	6×10^{-3}

Figure S1 The three-level nested domains setting in this work

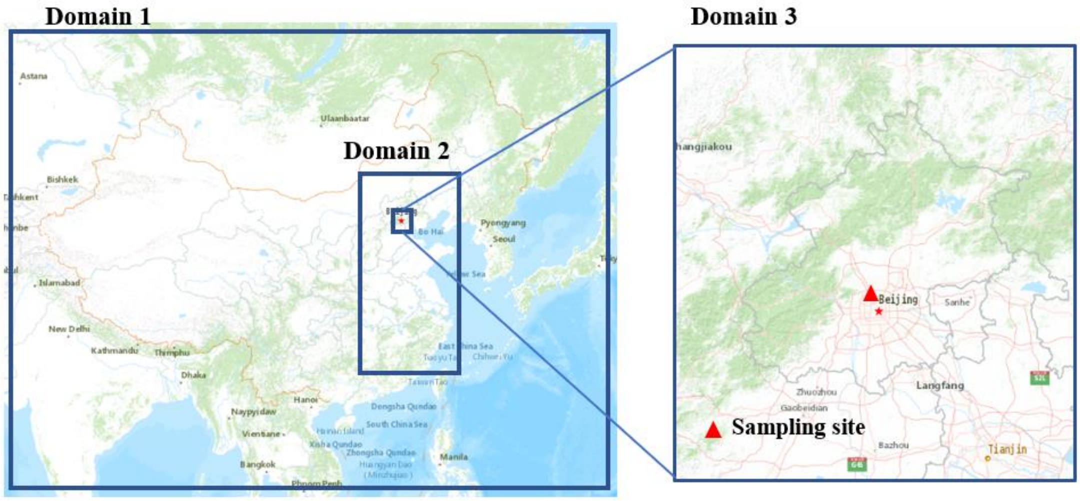

Figure S2 Spatial distribution of PCl emission in Beijing in 2017 (Unit: Kg/per grid).

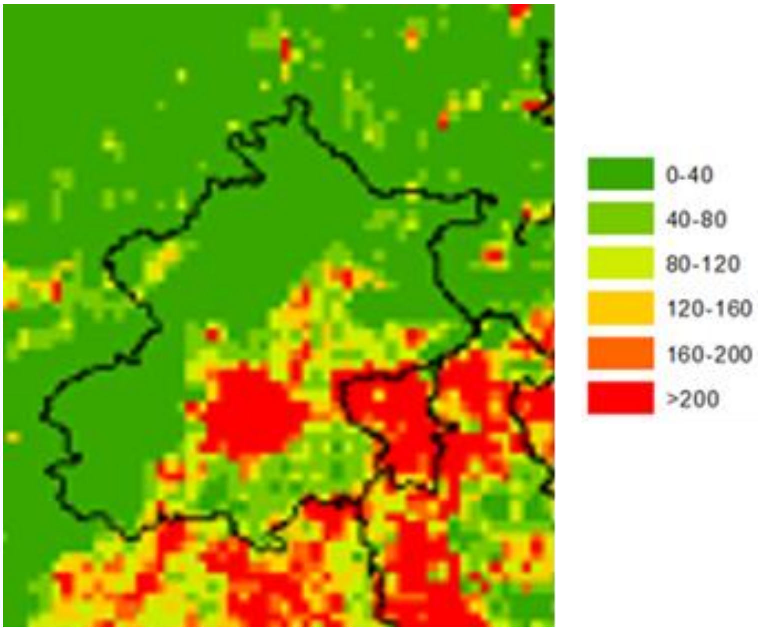

Figure S3 Spatial distributions of NO_2(a), O_3(b) and $PM_{2.5}$(c) concentrations averaged from 11 to 15 June 2017.

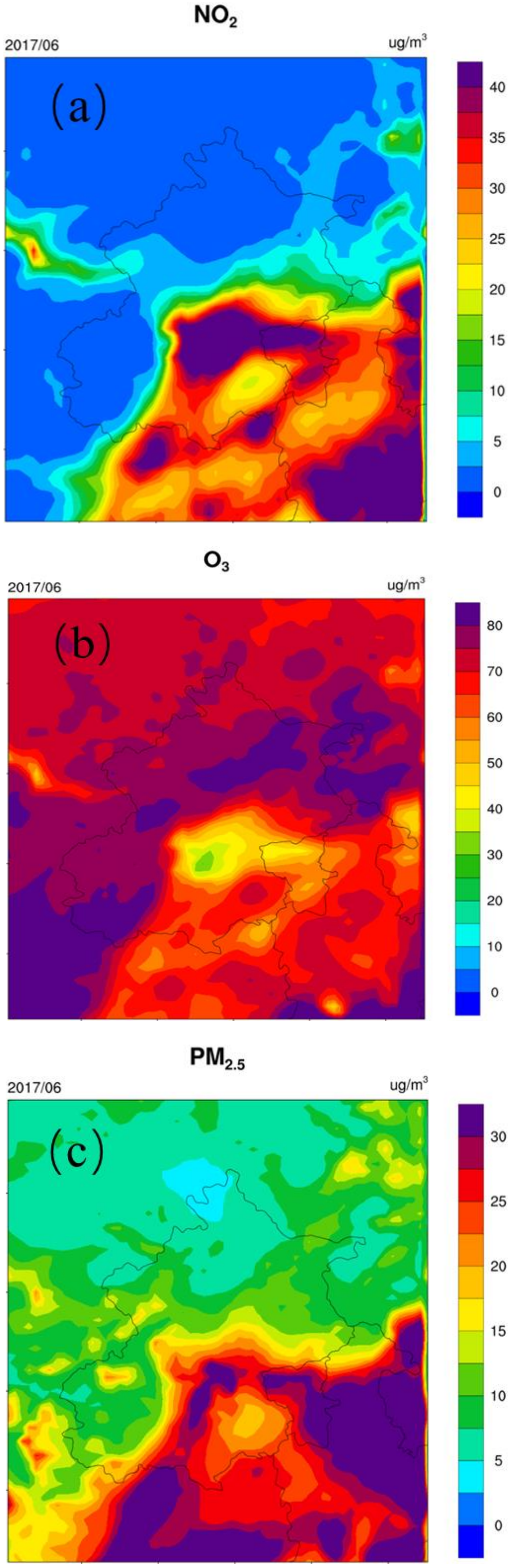

Figure S4 Spatial distributions of episode-average OH concentration (a) and the difference (b)((HET-BASE)/BASE) from 11 to 15 June 2017. Unit: 10^6 molecules cm^{-3}

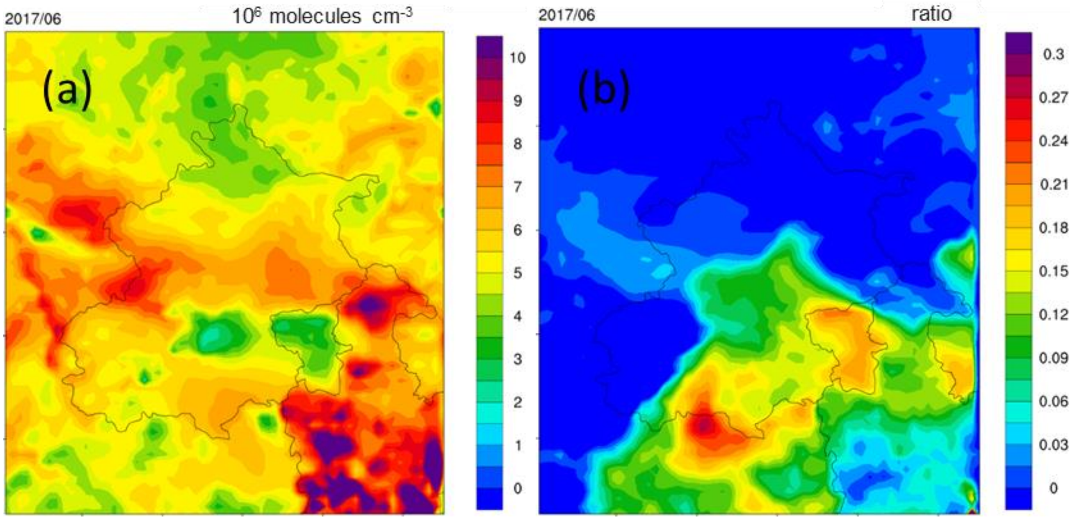

Figure S5 Spatial distribution of pH averaged from 11 to 15 June 2017.