Supporting information for:

Impacts of heterogeneous uptake of dinitrogen pentoxide and chlorine activation on ozone and reactive nitrogen partitioning: Improvement and application of WRF-Chem model in southern China

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Table S1. Mass fraction of elements in sea salt and dust

	In sea salt	In dust
Na	0.307	0.024
Cl	0.550	-
Ca	0.012	0.039
K	0.011	0.021
Mg	0.036	0.022

Table S2. The Cl initiated gaseous chemistry for RACM_ESRL mechanism.

No.	Reactions	Rate
RS01	Cl_2+hv=2.0 Cl	Photolysis rate of Cl_2
RS02	HOCl+hv=HO+Cl	Photolysis rate of HOCl
RS03	$ClNO_2$+hv=Cl+NO_2	Photolysis rate of $ClNO_2$
RS04	FMCl+hv=Cl+CO+HO_2	Photolysis rate of FMCl
RS05	HO+HCl=Cl+H_2O	(6.58D-13*EXP(58.0/TEMP)* (TEMP/300.0)**(1.16)) [a]
RS06	O_3+Cl=ClO{+O_2}	(2.3D-11*EXP(-200.0/TEMP))
RS07	ClO+ClO=0.3 Cl_2+1.4 Cl{+O_2}	1.63D-14
RS08	NO+ClO=Cl+NO_2	(6.4D-12*EXP(290.0/TEMP))
RS09	ClO+HO_2=HOCl{+O_2}	(2.7D-12*EXP(220.0/TEMP))
RS10	NO_2+Cl=$ClNO_2$	K_{RS10} [b]
RS11	CH_4+Cl=HCl+MO_2	(6.6D-12*EXP(-1240.0/TEMP))
RS12	ETH+Cl=HCl+0.991 ALD+XO_2+HO_2	(8.3D-11*EXP(-100.0/TEMP))
RS13	HC3+Cl=HCl+XO_2+0.11 HO_2+0.11 ALD	5.0D-11
RS14	HC5+Cl=HCl+XO_2+0.11 HO_2+0.11 ALD	5.0D-11
RS15	HC8+Cl=HCl+XO_2+0.11 HO_2+0.11 ALD	5.0D-11
RS16	ETE+Cl=FMCl+2.0 XO_2+HO_2+HCHO	1.07D-10
RS17	OLT+Cl=FMCl+ALD+2.0 XO_2+HO_2	2.5D-10
RS18	OLI+Cl=0.3 HCl+0.7 FMCl+ALD+0.3 OLT + 0.1 HC3+0.1 HC5+0.1 HC8+1.7 XO_2+HO_2	3.5D-10
RS19	ISO+Cl=0.15HCl+XO_2+HO_2+0.85FMCl+ISOP	4.3D-10
RS20	FMCl+HO=Cl+CO+H_2O	5.0D-13
RS21	HCHO+Cl=HCl+HO_2+CO	(8.2D-11*EXP(-34.0/TEMP))
RS22	ALD+Cl=HCl+ACO_3	1.05D-10
RS23	TOL+Cl=HCl+XO_2+0.88 HO_2	6.1D-11
RS24	XYL+Cl=HCl+XO_2+0.84 HO_2	1.2D-10

[a] TEMP is air temperature.

[b] $K_{RS10} = \frac{K_0[M]}{\left(1+\frac{K_0[M]}{K_\infty}\right)} F^Z$. $K_0 = 1.8 \times 10^{-31} \left(\frac{T}{300}\right)^{-2.0}$. $K_\infty = 1.0 \times 10^{-10} \left(\frac{T}{300}\right)^{-1.0}$. $F = 0.6$.

$Z = \frac{1.0}{1.0+(\log_{10}\left(\frac{K_0[M]}{K_\infty}\right))^{2.0}}$. [M] is the atmospheric pressure in molecules cm^{-3}.

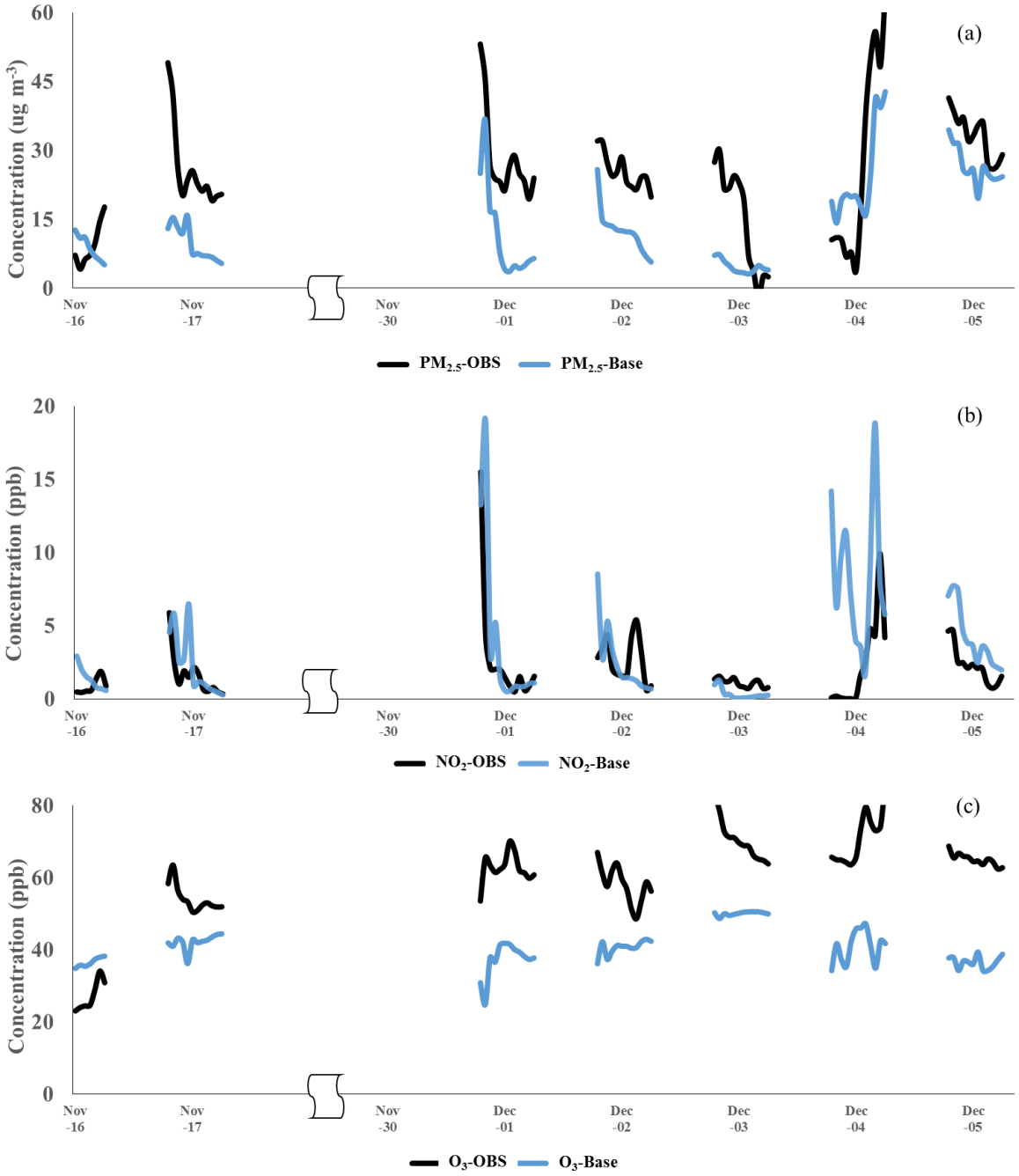

Figure S1. Hourly observed and simulated (Base case) (a) $PM_{2.5}$, (b) NO_2, and (c) O_3 concentrations at the nights when N_2O_5 and $ClNO_2$ were observed.

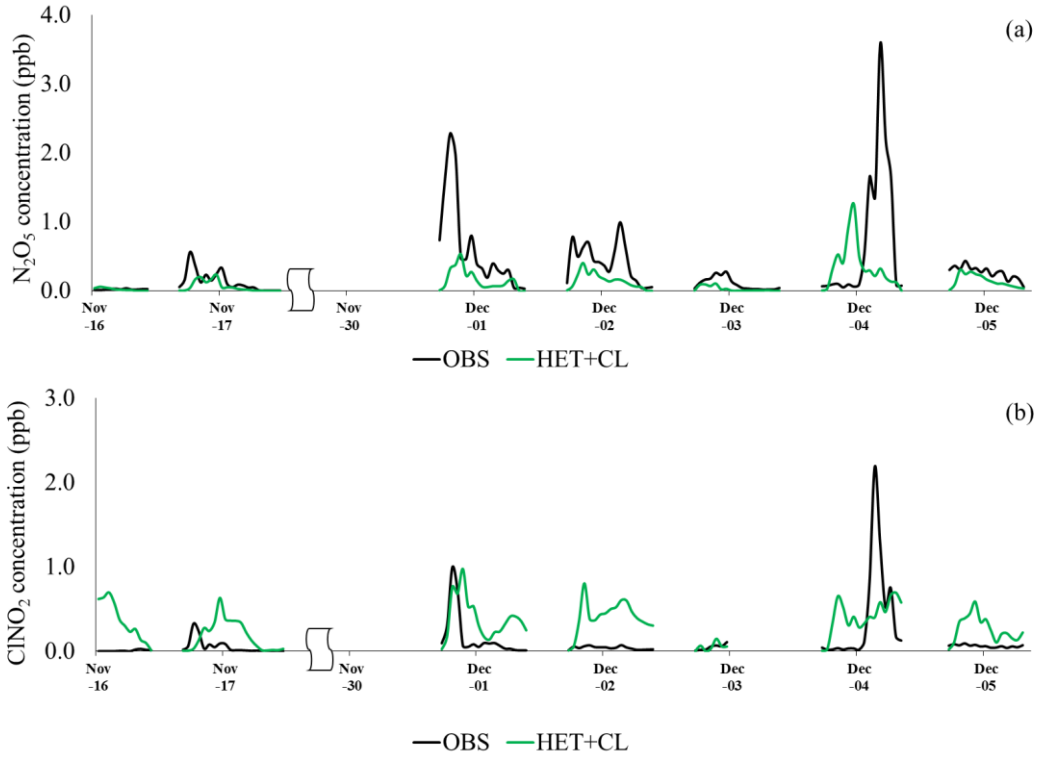

Figure S2. Hourly concentrations of observed and simulated (a) N_2O_5 and (b) $ClNO_2$ concentrations at TMS site.

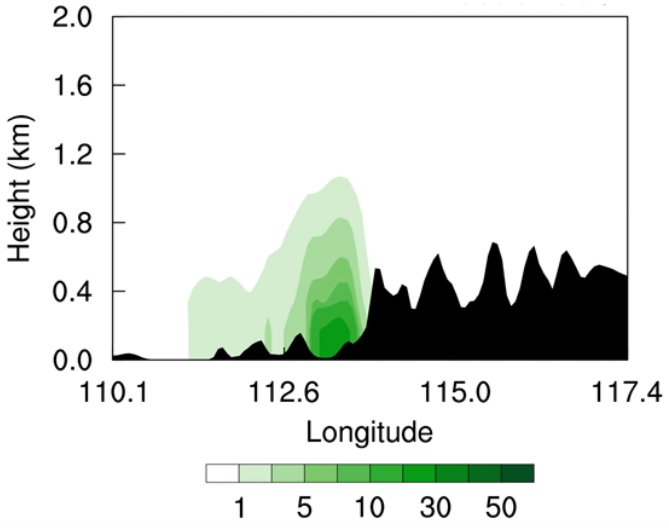

Figure S3. Vertical distributions of NO (ppb) average mixing ratios during the study period in the domain intercepting PRD and along the prevailing wind from Base case

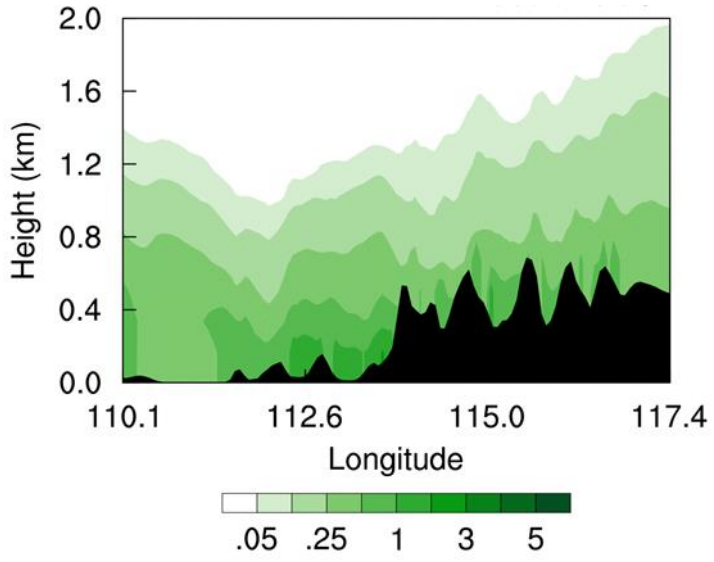

Figure S4. Vertical distributions of chloride (μg m^{-3}) average concentrations during the study period in the domain intercepting PRD and along the prevailing wind from Base case

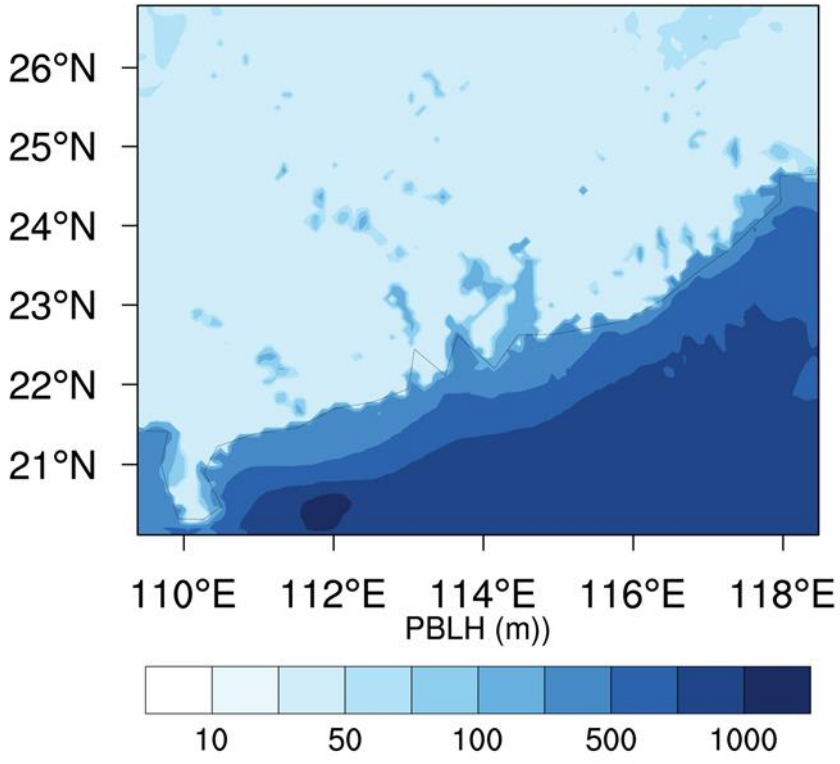

Figure S5. Boundary layer height in Southern China at 06:00 Dec 2, LT, as simulated in WRF-Chem

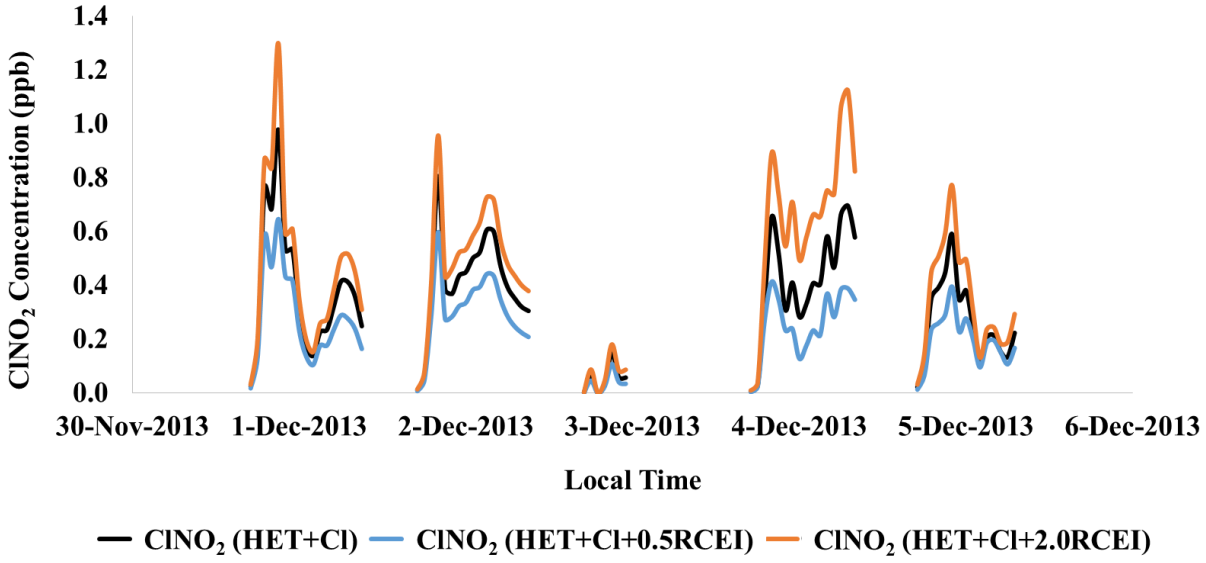

Figure S6. Hourly results of $ClNO_2$ concentrations from simulations with original, half and twice RCEI emission