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Supplement of

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

Qinyi Li et al.

Correspondence to: T. Wang (cetwang@polyu.edu.hk)

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

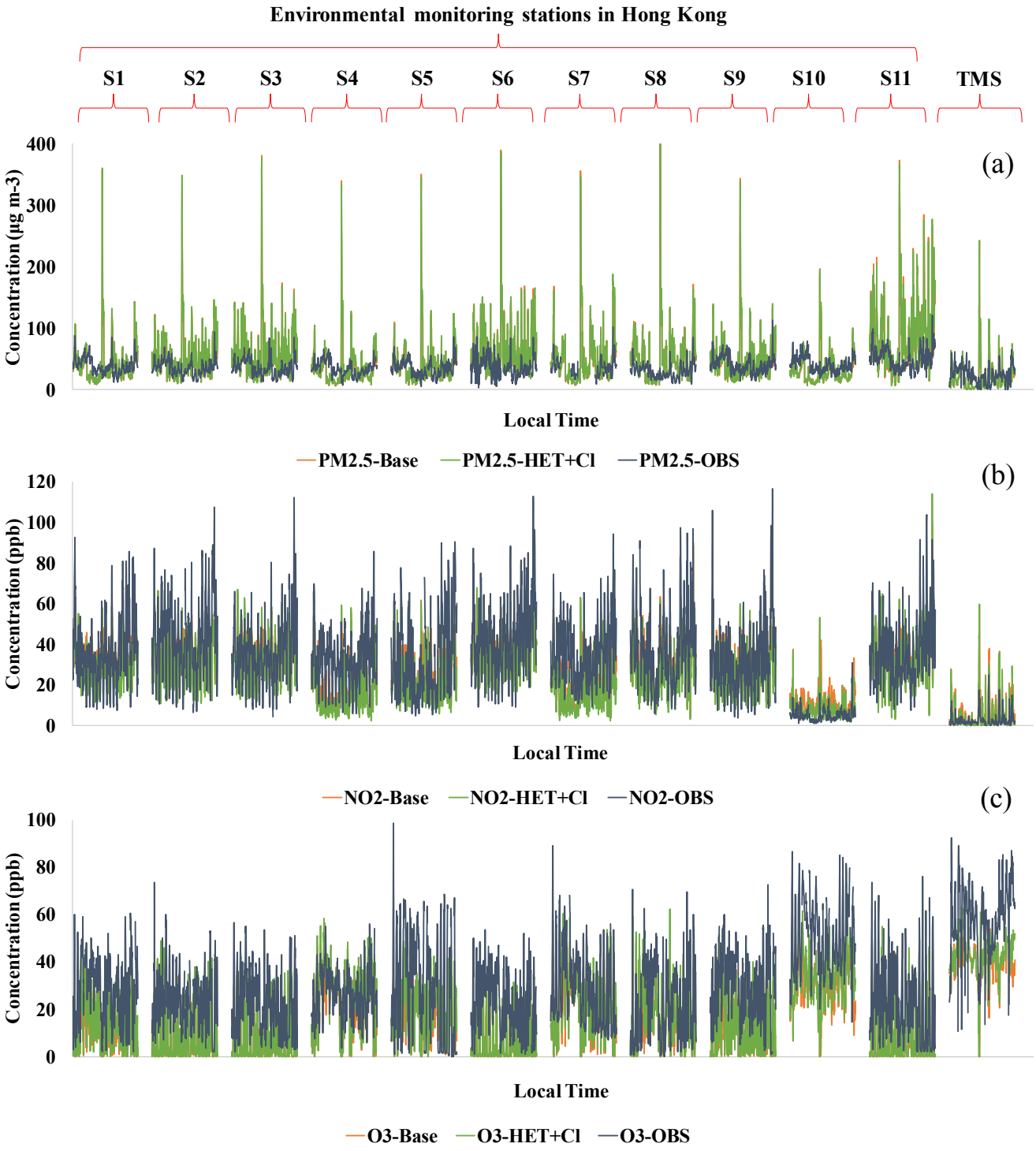
Table S2. The Cl initiated gaseous chemistry for RACM_ESRL mechanism.

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}.


Environmental monitoring stations in Hong Kong
S1
S2
S3
S4
S5
S6
S7
S8
S9
S10
S11
TMS
(a)
Concentration (μg m-3)
400
300
200
100
0
Local Time
PM2.5-Base
PM2.5-HET+Cl
PM2.5-OBS
(b)
Concentration (ppb)
120
100
80
60
40
20
0
Local Time
NO2-Base
NO2-HET+Cl
NO2-OBS
(c)
Concentration (ppb)
100
80
60
40
20
0
Local Time
O3-Base
O3-HET+Cl
O3-OBS

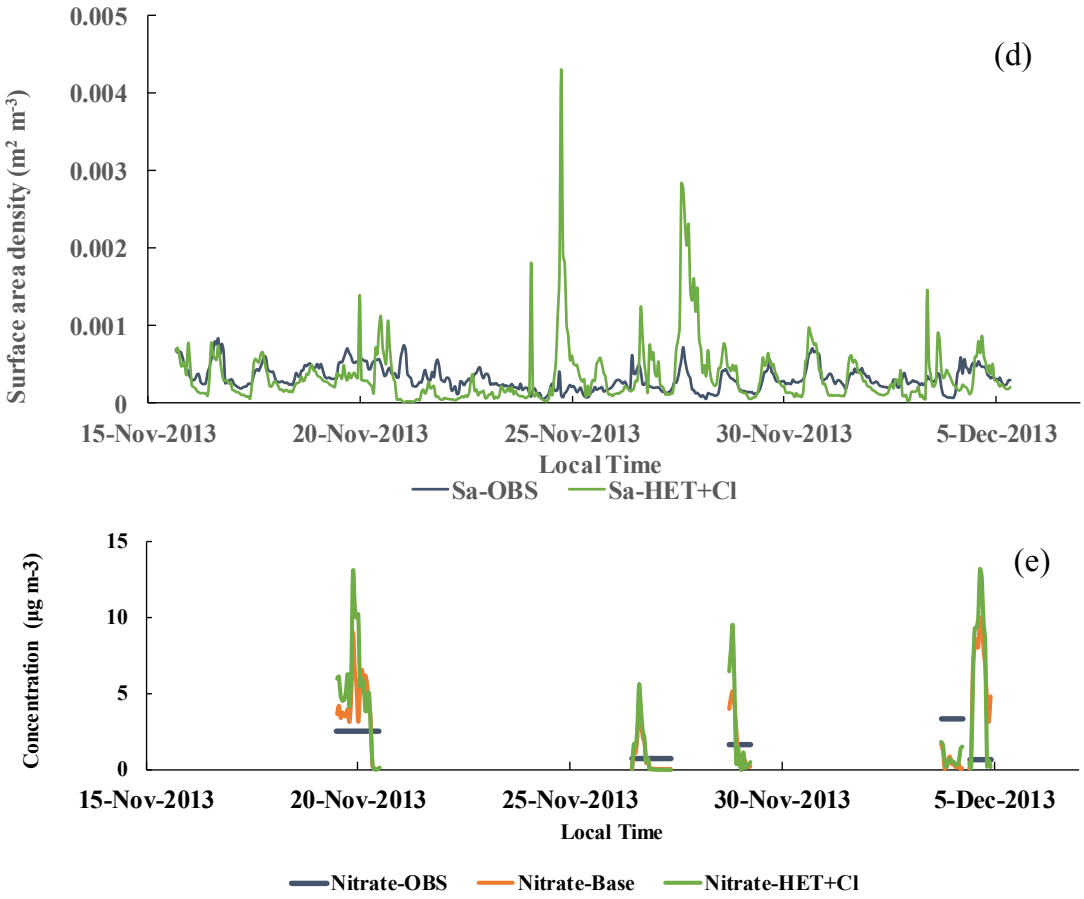


Figure S1. Hourly observed and simulated (Base case and HET+Cl case) (a) $PM_{2.5}$, (b) NO_2, and (c) O_3 concentrations during the entire simulation period at the monitoring stations and at TMS, and (d) surface area density and (e) nitrate concentration at TMS.

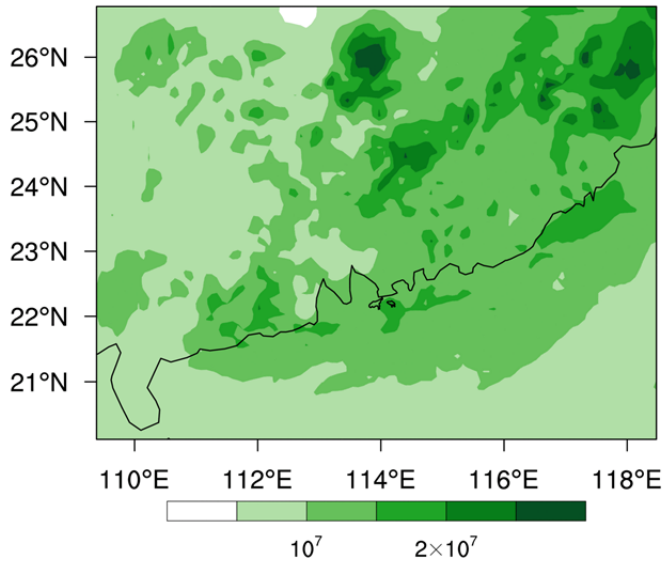


Figure S2. Average simulated ratio of surface area to volume (m^{-1}) for the particles within the PBL

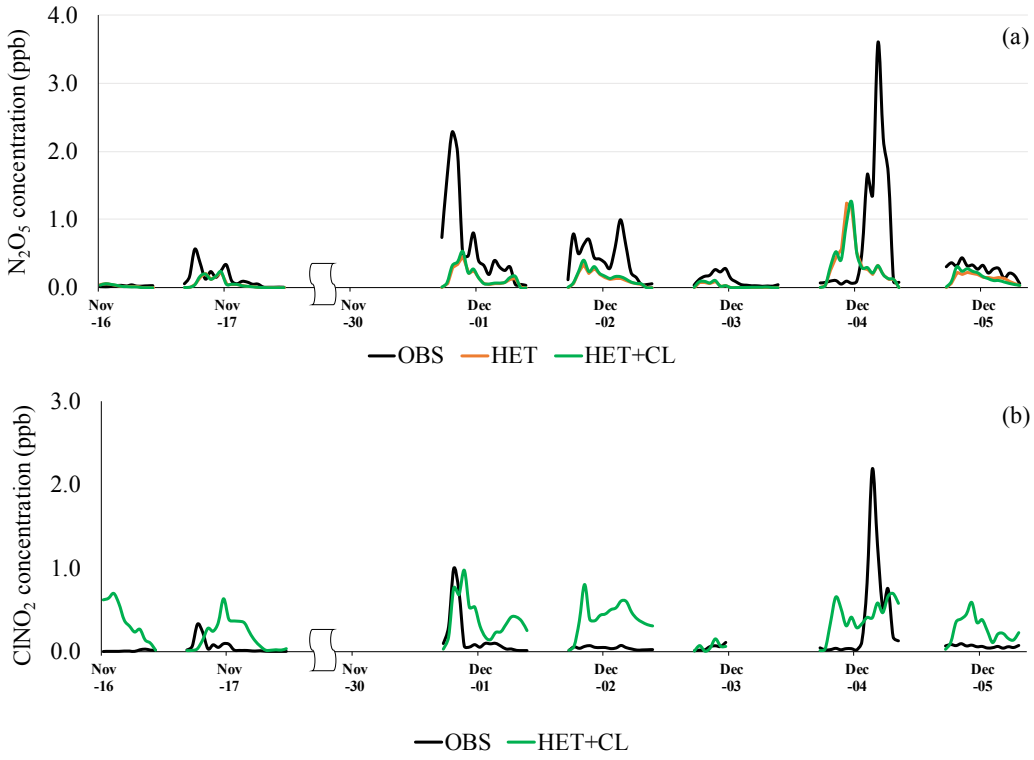


Figure S3. Hourly concentrations of observed and simulated (a) N_2O_5 and (b) $ClNO_2$ concentrations at TMS site.

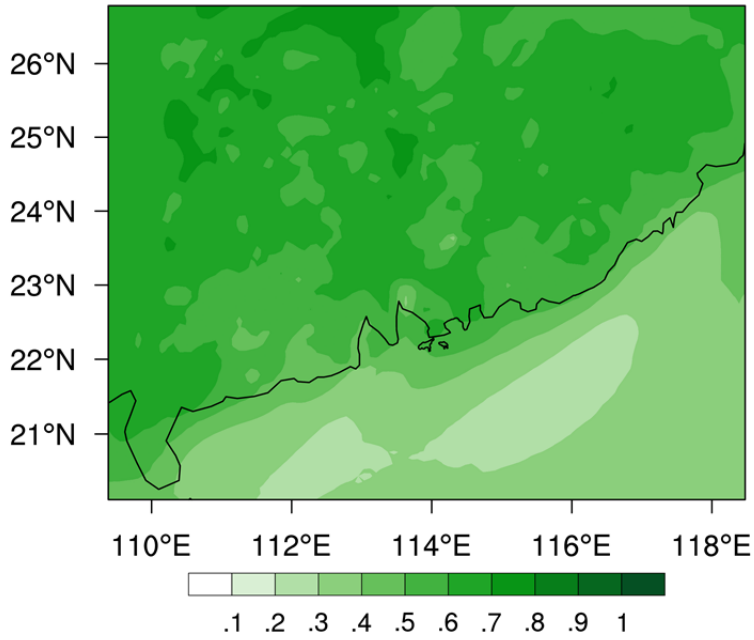


Figure S4. The average simulated yield of $ClNO_2$ within the PBL during the simulation period.

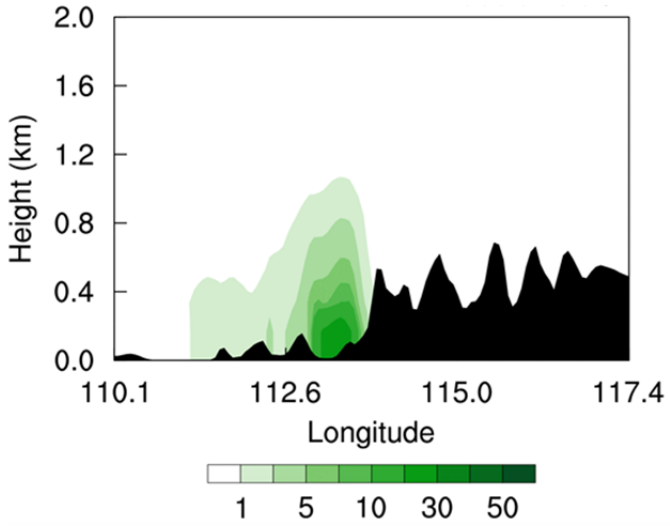


Figure S5. Vertical distributions of NO (ppb) average mixing ratios during the study period in the domain intercepting PRD and along the prevailing wind from Base case

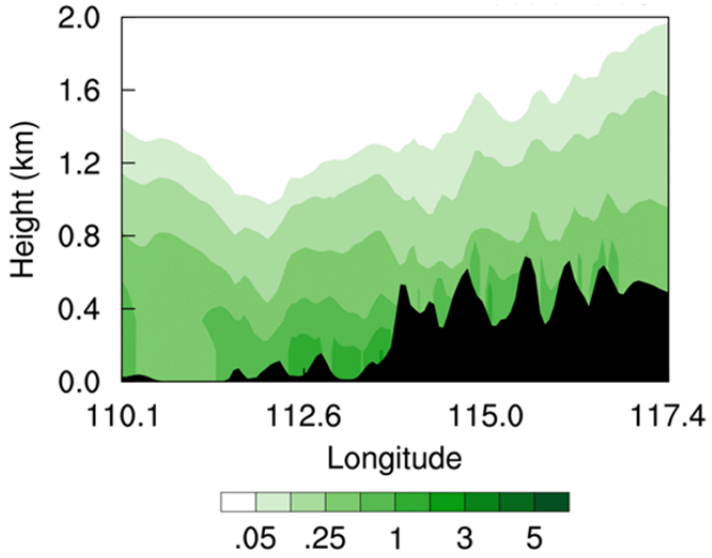


Figure S6. Vertical distributions of chloride (μg m^{-3}) average concentrations during the study period in the domain intercepting PRD and along the prevailing wind from Base case

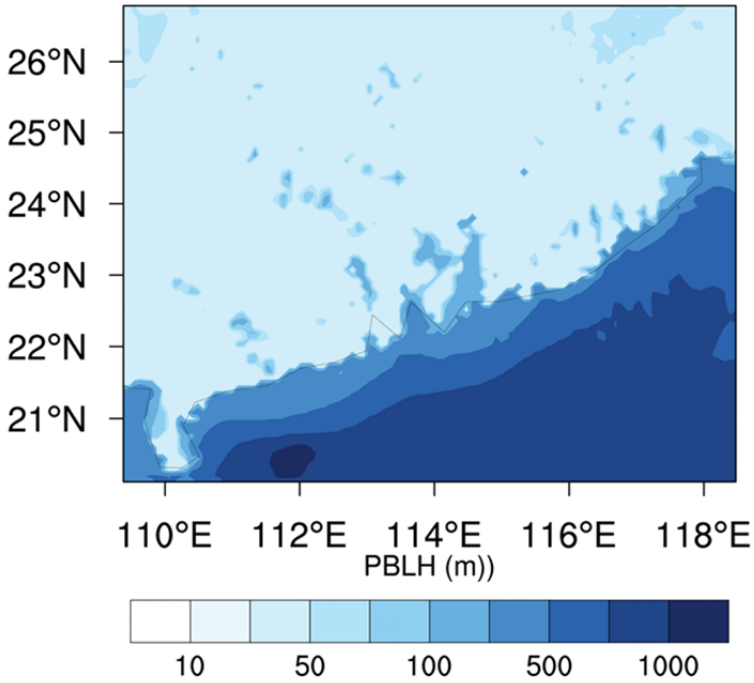


Figure S7. Boundary layer height in southern China at 06:00 Dec 2, LT, as simulated in WRF-Chem

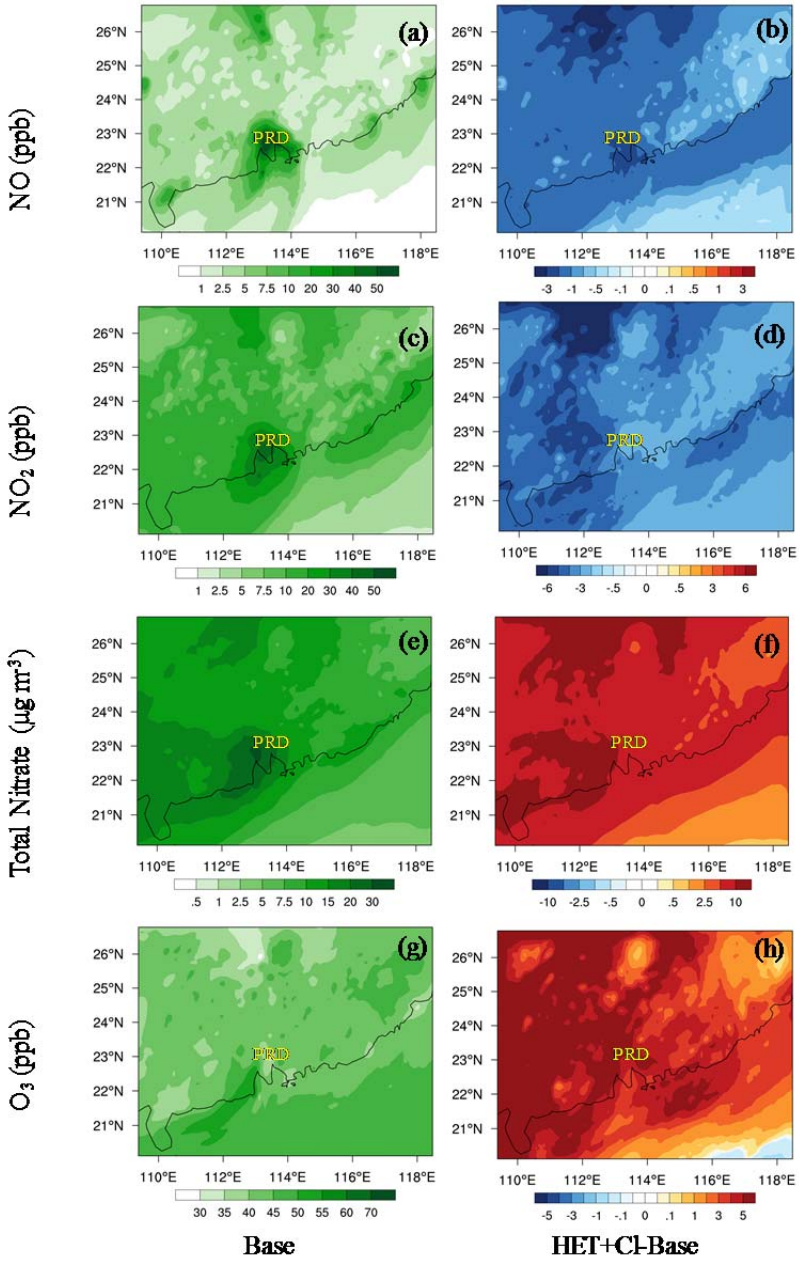


Figure S8. Horizontal distributions of average daily-maximum concentrations of (a) NO (ppb), (c) NO_2 (ppb), (e) total nitrate (μg m^{-3}) and (g) O_3 (ppb) during the study period within the PBL from Base case; the average impacts of N_2O_5 uptake and Cl activation on daily-maximum concentration of (b) NO (ppb), (d) NO_2 (ppb), (f) total nitrate (μg m^{-3}) and (h) O_3 (ppb) during the simulation period in the horizontal domain within the PBL.

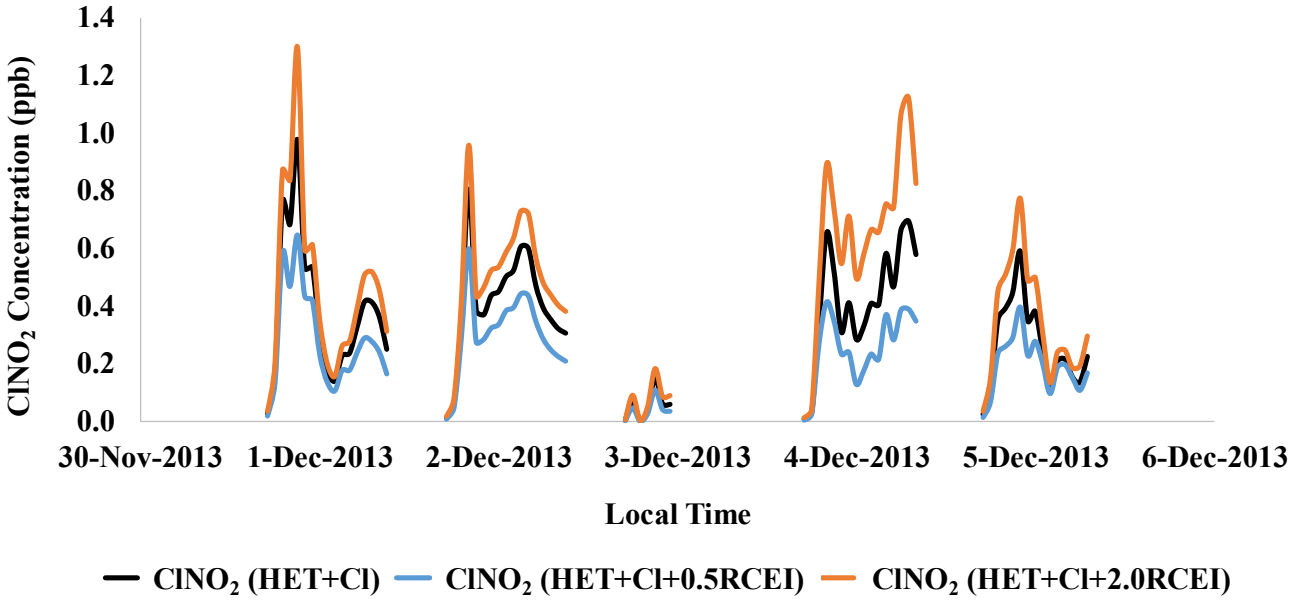


Figure S9. Hourly results of $ClNO_2$ concentrations from simulations with original, half and twice RCEI emission