



Supplement of

Combined impacts of nitrous acid and nitryl chloride on lower-tropospheric ozone: new module development in WRF-Chem and application to China

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Region	Case	No. OBS	OBS ^a	MOD	COR	MB	RMSE	NMB	NME
NCP	BASE	48362	10.4	18.4	0.35	-1.0	16.3	-5.0%	58.6%
	ReNOM		19.4	14.4	0.35	-5.0	15.8	-25.8%	56.3%
YRD	BASE	35421	177	27.0	0.21	9.3	23.5	52.3%	96.9%
	ReNOM		1/./	19.2	0.17	1.4	17.9	8.1%	75.8%
PRD	BASE	15651	10.1	8.3	0.38	-3.9	11.9	-31.8%	71.5%
	ReNOM		12.1	7.2	0.35	-5.0	11.5	-40.8%	69.7%
China	BASE	213308	15.0	14.2	0.32	-1.4	16.3	-9.2%	73.1%
	ReNOM		15.0	10.9	0.32	-4.8	14.6	-30.5%	67.4%

Table S1. Statistics of model performance in the base and ReNOM cases for hourly NO_2 measurements (ppb) at the MEP air quality monitoring stations during the simulation period (27 Jun-7 Jul 2014).

Region	Case	No. OBS	OBS_scaled ^a	MOD	COR	MB	RMSE	NMB	NME
NCP	BASE	48362	15.6	18.4	0.48	2.8	14.4	17.9%	62.2%
	ReNOM		13.5	14.4	0.51	0.9	11.7	6.9%	57.6%
YRD	BASE	35421	14.4	27.0	0.37	12.6	23.3	87.3%	113.9%
	ReNOM		11.7	19.2	0.38	7.5	16.6	64.4%	92.7%
PRD	BASE	15651	10.0	8.3	0.37	-1.7	11.0	-17.1%	77.0%
	ReNOM		8.1	7.2	0.42	-0.9	9.1	-11.5%	75.3%
China	BASE	213308	12.3	14.2	0.43	1.9	14.7	15.2%	77.6%
	ReNOM		10.5	10.9	0.45	0.4	11.3	3.7%	70.7%

^a OBS: original observations of NO₂; OBS_scaled: scaled observations of NO₂ based on model simulated reactive nitrogen species by using the equation of $NO_2 \ _{obs} = NO_2^* \ _{obs} \times \frac{NO_2 \ _{mod}}{NO_2 \ _{mod} + NO_2 \ _{mod} - Nitrate_{mod}}$, where NO₂*_{obs} is the original measurement of NO₂, NO_{2 mod} is the model simulation of NO₂, NO_{2 mod} is the sum of simulations of HONO, 2×N₂O₅, CINO₂, CIONO₂, NO₃,

HNO₃, HNO₄, PAN, and Nitrate, Nitrate $_{mod}$ is the simulated nitrate; gas-phase HNO₃ is assumed to be converted into NO by 80% in the Mo converter due to its possible loss on inlet; other gas-phase NO_Z species are assumed to be converted by 100%.

Species	OBS	BASE	ReNOM_Cl	ReNOM_HONO	ReNOM				
CO (ppb)	541.0	577.4	578.4	572.3	574.2				
SO ₂ (ppb)	7.7	8.1	8.0	7.9	7.9				
NO ₂ (ppb)	12.8	13.5	12.4	11.4	10.7				
O ₃ (ppb)	55.6	51.5	54.6	55.5	56.5				
$PM_{2.5} (\mu g/m^3)$	84.9	90.5	101.6	96.8	106.6				
HONO (ppt)	941.2	38.5	37.2	769.4	805.3				
$N_2O_5(ppt)$	28.0	/	28.0	/	23.9				
ClNO ₂ (ppt)	159.5	/	279.3	/	265.6				

Table S2. Observed and simulated major pollutants obtained from the CareBeijing 2014 campaign at Wangdu during the simulated period.



Figure S1. Spatial distributions of the (a) observed daily-averaged NO_2 concentration (ppb); (b) scaled observed daily-averaged NO_2 ; and modeled ones in (c) the Base case and (d) ReNOM case during the simulation period. The region of eastern China is highlighted with red box. Scaled observed NO2 was calculated based on the model simulations in the ReNOM case by using the

equation of $NO_{2 \ obs} = NO_{2 \ obs}^* \times \frac{NO_{2 \ mod}}{NO_{2 \ mod} + NO_{z \ mod} - Nitrate_{mod}}$.



Figure S2. (a) Spatial and (b) vertical distributions of nighttime chloride ($\mu g m^{-3}$) during the simulation period.



Figure S3. Observed and simulated (a) NO_2 , (b) HONO, (c) N_2O_5 and (b) $CINO_2$ at the Wangdu site during the simulation period (27 Jun - 7 Jul 2014). The NO_2 and HONO data are adopted from Tan et al. (2017).



Figure S4. Vertical distributions of daytime ozone enhancements in (a) ReNOM_HONO case, (b) ReNOM_Cl case, and (c) ReNOM case in the domain intercepting the northern China and central China. Vectors present the average v-w wind components (m s^1), dash lines the temperature (°C), and black line the simulated planetary boundary layer height during daytime.



Figure S5. Regional averages of NO_y partitioning over eastern China in (a) BASE case, (b) ReNOM_Cl case, (c) ReNOM_HONO case, and (d) ReNOM case.