Supplement of

Response relationship between atmospheric O_3 and its precursors in Beijing based on smog chamber simulation and a revised MCM model

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Calculation process of Normalized Mean Bias (NMB):

$$\mathrm{NMB} = \frac{\sum_{i=1}^{n}(P_i - O_i)}{\sum_{i=1}^{n} O_i} \times 100\ \%$$

P represents the simulated value, and O denotes the measured value.

NMB is a commonly used indicator for evaluating the performance of atmospheric models. It is mainly used to quantify the direction and magnitude of the systematic deviation of model simulated values relative to measured values. NMB also conducts the comparison of discrepancies between different data or different models through standardization processing (Zheng et al., 2024; Xuan et al., 2024).

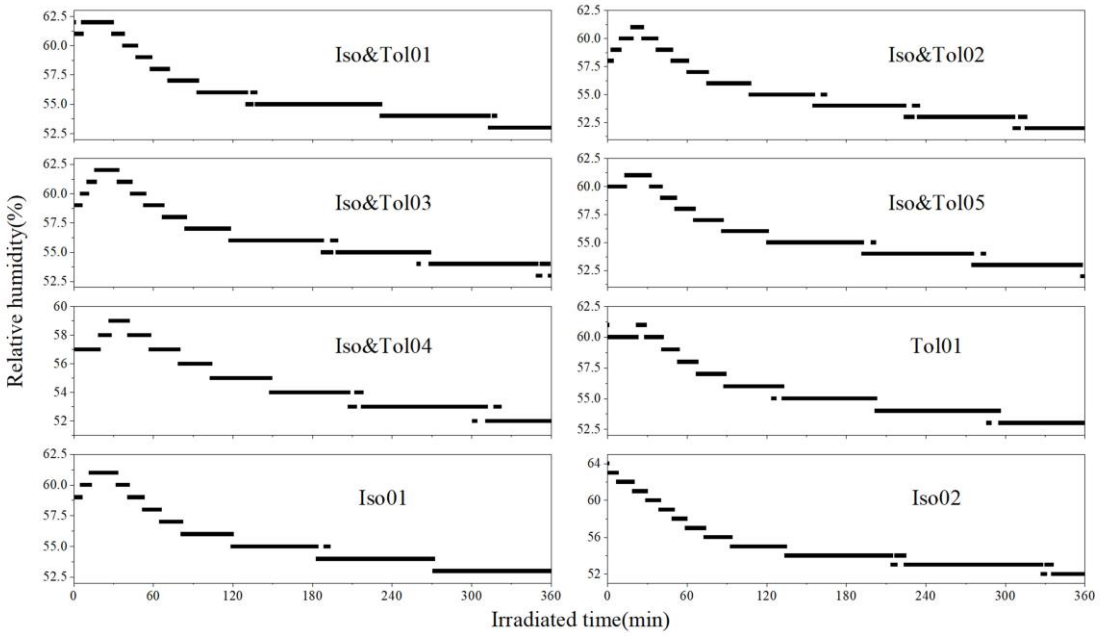

Figure S1: Variations in relative humidity of smog chamber during the experimental process.

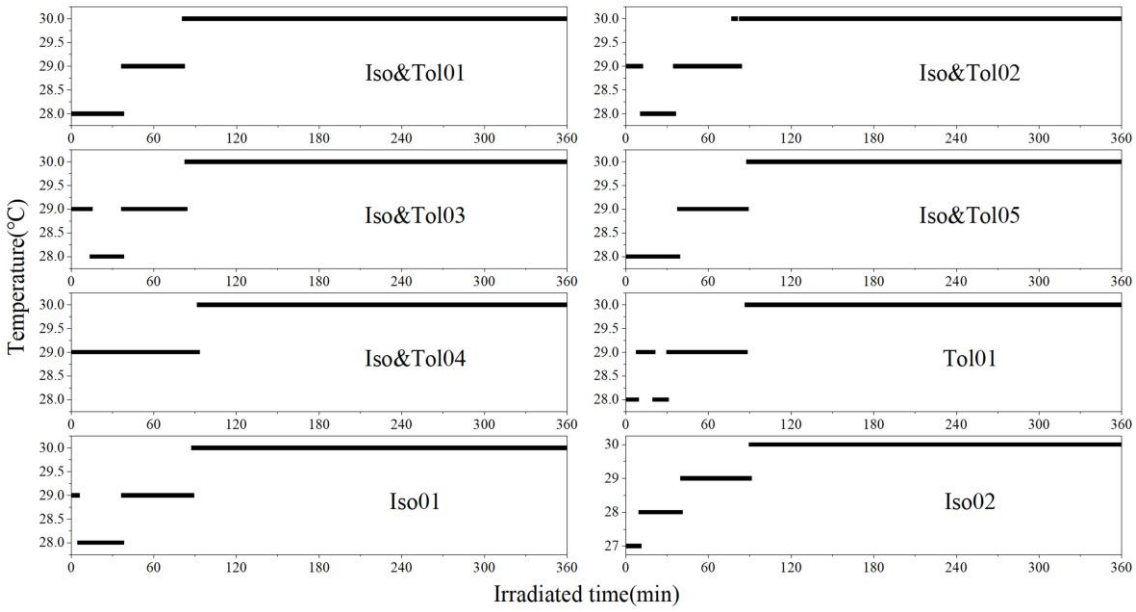

Figure S2: Variations in temperature of smog chamber during the experimental process.

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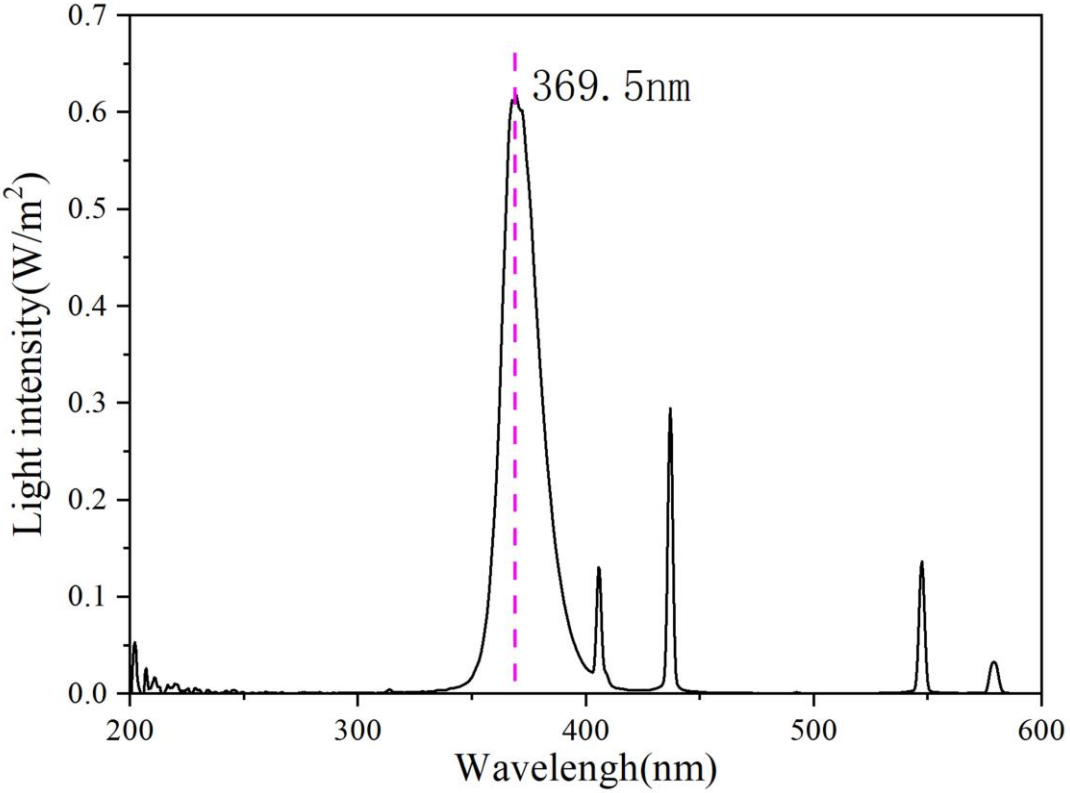

Figure S3: The ultraviolet spectra during the smog chamber experiments.

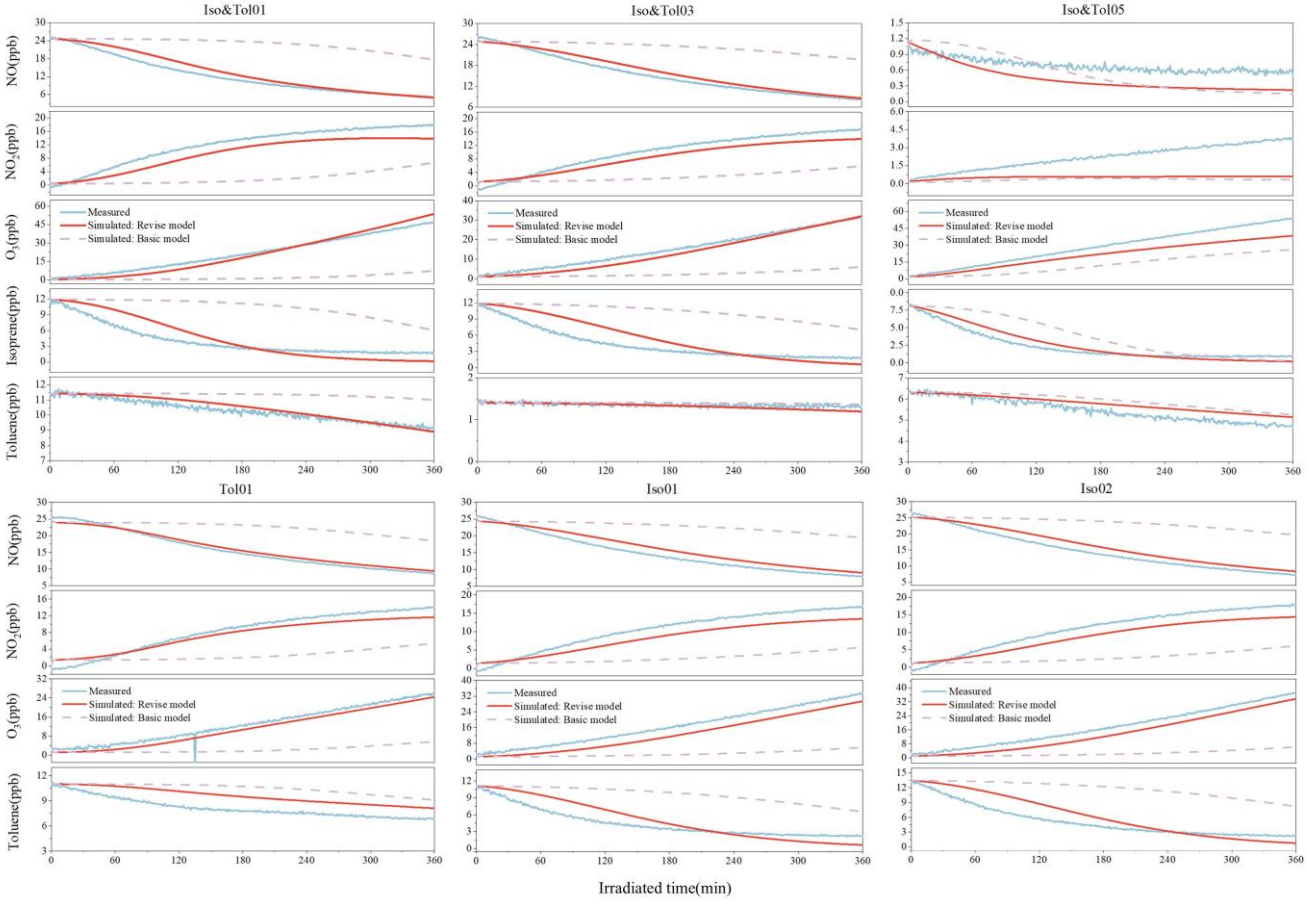

Figure S4: Time series of NO, NO_2, O_3, and VOCs concentrations during the photochemical reaction process in different experiments. The curves in different colors corresponding to the measured concentrations, the results from the basic model simulation, and the results from the revised model simulation. The NMB values for O_3 simulated by the basic model in experiments Iso&Tol01, Iso&Tol03, Iso&Tol05, Tol01, Iso01 and Iso02 were -91.1 %, -83.9 %, -56.9 %, -81.9 %, -84.4 % and -85.7 %, respectively. And that simulated by the revised model were -3.8 %, -12.5 %, -26.6 %, -13.8 %, -24.1 % and -21.6 %, respectively.

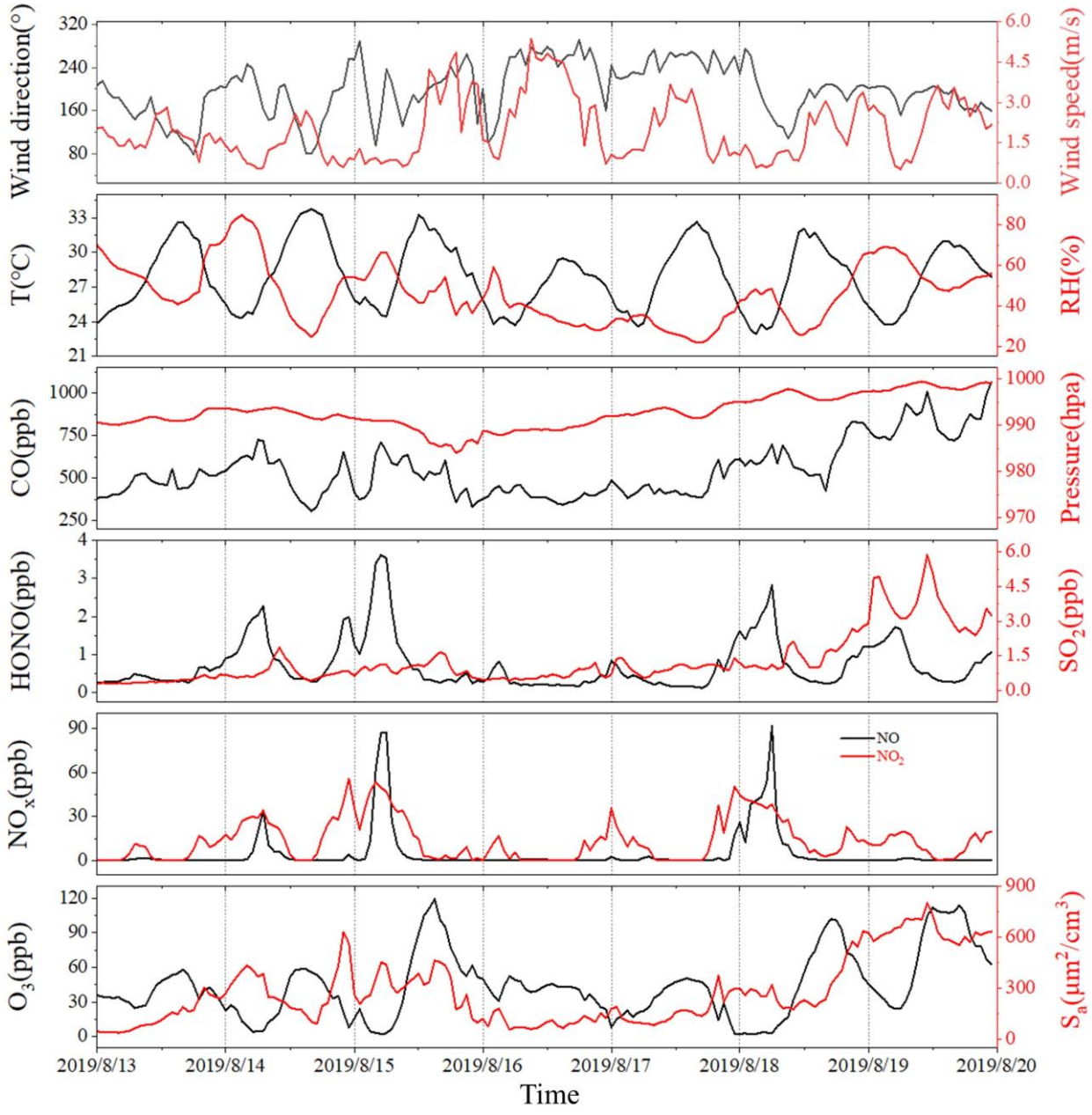

Figure S5: Time series of observed species concentrations and meteorological parameters in Daxing, Beijing from August 13–19, 2019.

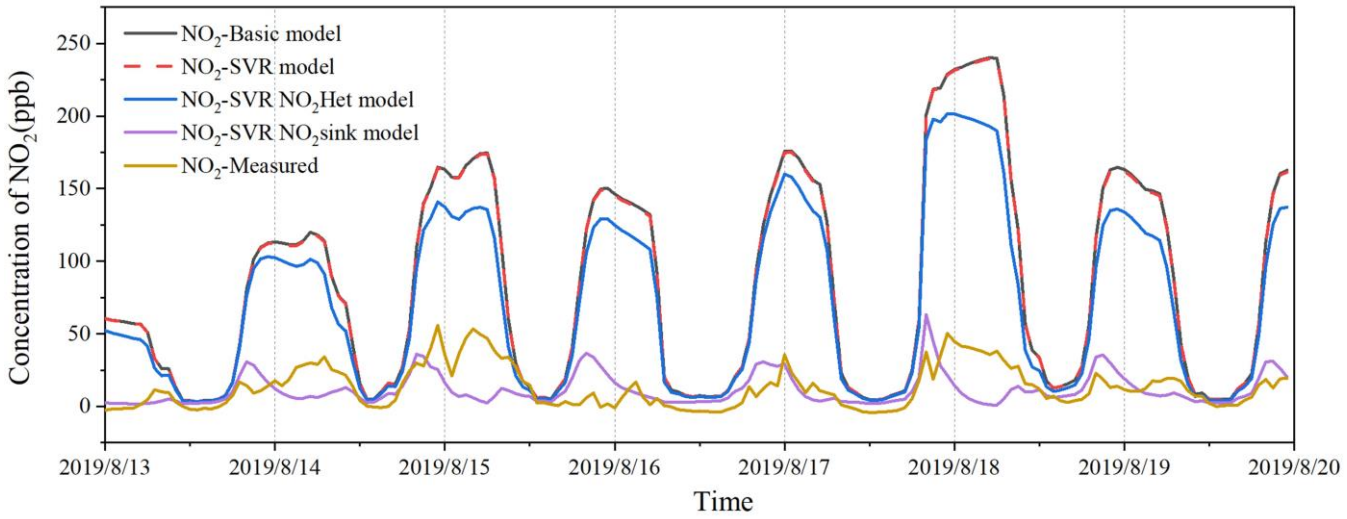

Figure S6: Measured concentrations of NO_2 and the simulation results of different models in Daxing, Beijing from August 13–19, 2019. The NMB values for NO_2 simulated by the Basic model, SVR model, SVR NO_2Het model, and SVR NO_2sink model were 539.8 %, 536.7 %, 436.7 % and -13.3 %, respectively.

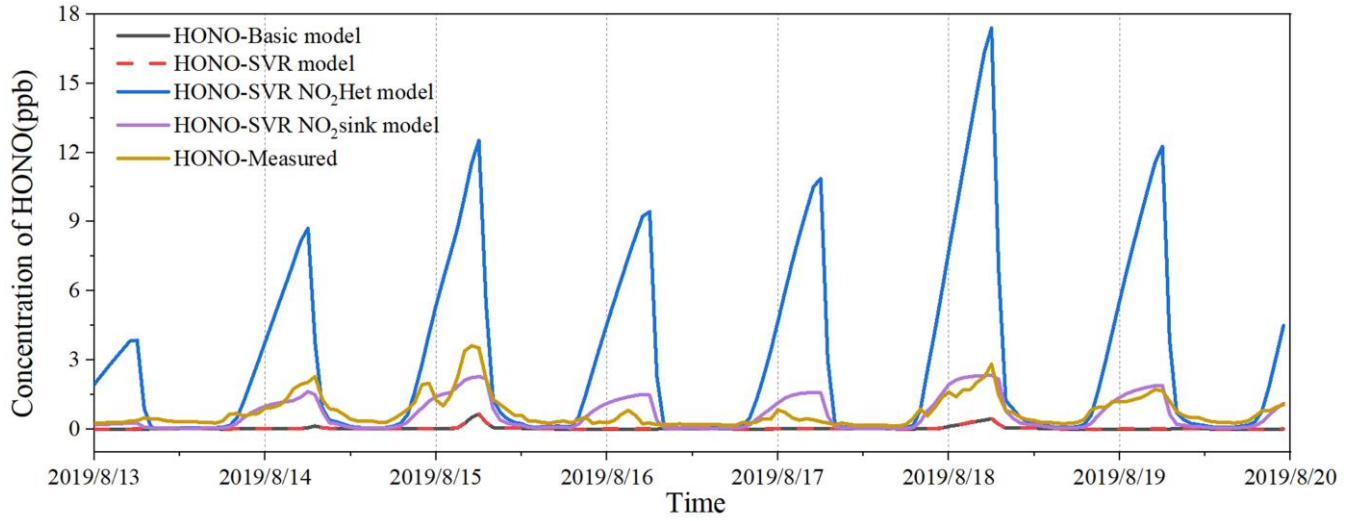

Figure S7: Measured concentrations of HONO and the simulation results of different models in Daxing, Beijing from August 13–19, 2019. The NMB values for HONO simulated by the Basic model, SVR model, SVR NO_2Het model, and SVR NO_2sink model were -94.8 %, -94.3 %, 305.6 % and -12.4 %, respectively.

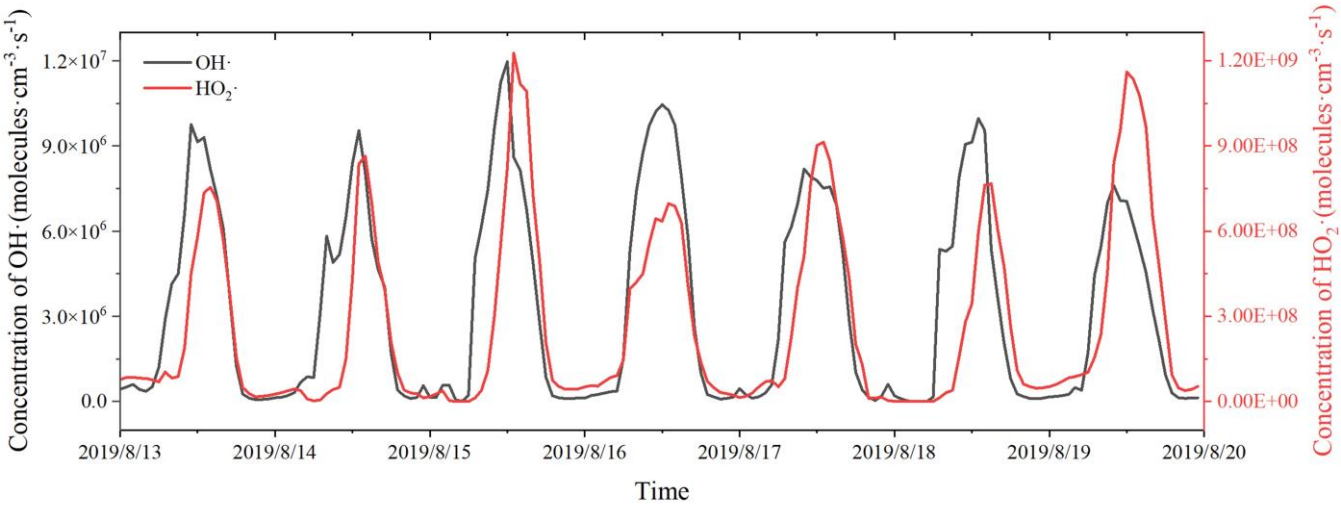

Figure S8: Simulated concentrations of OH and HO_2 radicals by SVR NO_2sink model in Daxing, Beijing from August 13–19, 2019.

Table S1: Photolysis rate constants used in the MCM box model for simulating smog chamber experiments.

J1	1.05E-05	J2	2.52E-06	J3	4.85E-06
J4	9.20E-03	J5	2.17E-05	J6	5.37E-05
J7	2.03E-03	J8	5.66E-07	J11	1.94E-06
J12	2.20E-06	J13	9.73E-07	J14	1.61E-06
J15	5.20E-07	J16	2.48E-07	J17	2.31E-06
J18	5.12E-07	J19	5.12E-07	J20	2.63E-04
J21	3.10E-07	J22	2.81E-07	J23	3.08E-07
J24	3.08E-07	J31	5.62E-07	J32	5.17E-06
J33	3.24E-05	J34	3.85E-05	J35	7.34E-05
J41	4.56E-07	J51	9.22E-07	J52	1.76E-07
J53	2.71E-04	J54	2.86E-04	J55	1.08E-06
J56	7.26E-06				

Table S2: Constrained species in AtChem2-MCM.

Parameters category	Parameters
Trace species	NO, CO, SO_2
Photolysis frequency	J4
Meteorology	TEMP, PRESS, RH, ASA
VOCs	HCHO, CH3CHO, C3H6, C4ALDB, C2H5CHO, C5H8, TM123B, C4H6, C3H7CHO, MXYL, CCL2CH2, TOLUENE, C4H9CHO, CH3COCH3, VINCL, C5H11CHO, NC4H10, PENT1ENE, NC11H24, HEX1ENE (name in MCM)

References

Xuan, H., Liu, J., Zhao, Y., Cao, Q., Chen, T., Wang, Y., Liu, Z., Sun, X., Li, H., Zhang, P., Chu, B., Ma, Q., and He, H.: Relative humidity driven nocturnal HONO formation mechanism in autumn haze events of Beijing, npj Climate and Atmospheric Science, 7, 193, 10.1038/s41612-024-00745-8, 2024.

Zheng, H., Gen, M., Sun, Y., Xu, W., Ma, N., Su, H., Cheng, Y., Wang, S., Xing, J., Zhang, S., Xue, L., Xue, C., Mu, Y., Tian, X., Matsuki, A., and Song, S.: Rapid hydrolysis of NO_2 at High Ionic Strengths of Deliquesced Aerosol Particles, Environmental Science & Technology, 58, 7904-7915, 10.1021/acs.est.3c08810, 2024.