

Supplementary information of

Heterogeneous Uptake of N₂O₅ In Sand Dust and Urban Aerosols Observed During the Dry Season in Beijing

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Text S1: Input and configuration of the E-AIM model.

E-AIM model was run online at <http://www.aim.env.uea.ac.uk/aim/model3/model3a.php> to obtain aqueous phase [H₂O], [Cl⁻] and [NO₃⁻]. The batch mode of Model III was used. Input data include RH, NH₄⁺, Na⁺, SO₄²⁻, NO₃⁻ and Cl⁻. Model configurations are shown below. Parameter e=1, meaning that water dissociation will be considered. Parameter p, q, r, s=3, which assumes that the evaporation of HNO₃ (g), HCl (g), NH₃ (g) and H₂SO₄ (g) did not occur. Parameter u=0, which means that the model allowed the formation of solids.

Table S1: measured VOCs species and reaction rate constants with NO₃ radical at 298 K. TMB is the abbreviation of trimethylbenzene.

Species	$k(298K)$ cm ³ molecule ⁻¹ s ⁻¹	Species	$k(298K)$ cm ³ molecule ⁻¹ s ⁻¹
Alkanes		Aromatic hydrocarbons	
ethane	1×10 ⁻¹⁷	benzene	3×10 ⁻¹⁷
propane	7×10 ⁻¹⁷	toluene	7×10 ⁻¹⁷
n-butane	4.59×10 ⁻¹⁷	ethylbenzene	6×10 ⁻¹⁶
n-pentane	8.7×10 ⁻¹⁷	o-xylene	4.1×10 ⁻¹⁶
cyclopentane	1.4×10 ⁻¹⁶	m&p-xylene	3.8×10 ⁻¹⁶
n-hexane	1.1×10 ⁻¹⁶	1,2,3-TMB	1.9×10 ⁻¹⁵
2-methylpentane	1.8×10 ⁻¹⁶	1,2,4-TMB	1.8×10 ⁻¹⁵
3-methylpentane	2.2×10 ⁻¹⁶	1,3,5-TMB	8.8×10 ⁻¹⁶
2,2-dimethylbutane	4.4×10 ⁻¹⁶	styrene	1.5×10 ⁻¹²
2,3-dimethylbutane	4.4×10 ⁻¹⁶	n-propylbenzene	1×10 ⁻¹⁵
cyclohexane	1.4×10 ⁻¹⁶		
n-heptane	1.5×10 ⁻¹⁶	Biogenic VOCs	
2-methylhexane	1.8×10 ⁻¹⁶	isoprene	7.0×10 ⁻¹³
3-methylhexane	1.8×10 ⁻¹⁶	α-pinene	6.16×10 ⁻¹²
2,4-			
dimethylpentane	1.5×10 ⁻¹⁶	β-pinene	2.51×10 ⁻¹²
n-octane	1.9×10 ⁻¹⁶		
2,2,4-			
trimethylpentane	9×10 ⁻¹⁷		
Alkenes			

ethene	2.05×10^{-16}
propene	9.49×10^{-15}
1-butene	1.35×10^{-14}
<i>cis</i> -2-butene	3.52×10^{-13}
<i>trans</i> -2-butene	3.9×10^{-13}
1-pentene	1.5×10^{-14}
1,3-butadiene	1.0×10^{-13}
<i>trans</i> -2-pentene	3.9×10^{-13}
<i>cis</i> -2-pentene	3.5×10^{-13}

Figure S1: Backward trajectories of the air masses mentioned in the main text (Figure 4 and Table 1). The model was run online at <https://ready.arl.noaa.gov/HYSPLIT.php>. Dates colored in orange represent light dust or heavy sand storm events, while dates colored in blue denote urban air masses. The input information is shown below. Meteorology: GDAS (0.5 degree, global, 09/2007–present). Starting location: 40.04 N, 116.42 E. Starting time: local time 04:00. Total run time: 24 h. Height: 200 m (red line), 500 m (blue line), 1000 m (green line). Zoom factor: 70.

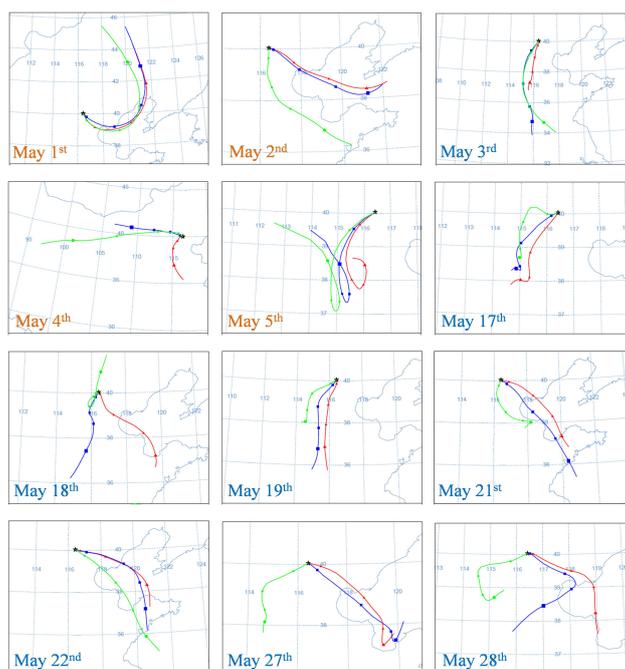


Figure S2: Dependence of N_2O_5 sensitivity on RH determined on site during the field campaign. The fitted curve ($y=0.235+2.613x-2.872x^2$) was used to correct the humidity effect on ambient N_2O_5 data.

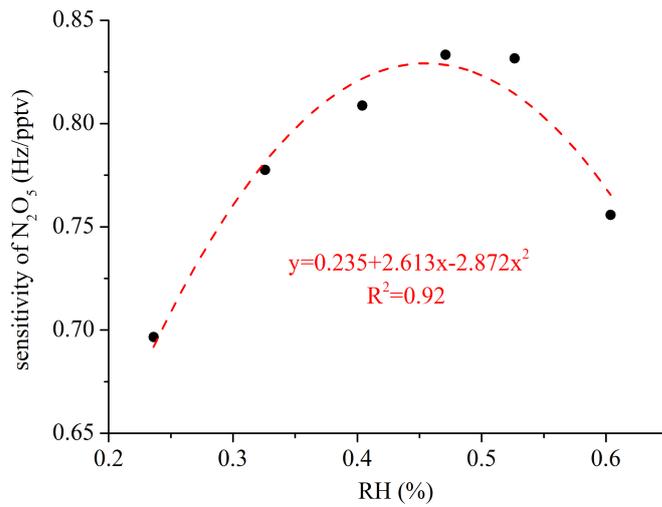


Figure S3: Average diurnal patterns of N_2O_5 , $ClNO_2$, and related species. **(a)** the early part of the campaign from Apr 24th to May 13th. **(b)** The latter part of the campaign from May 14th to May 31st.

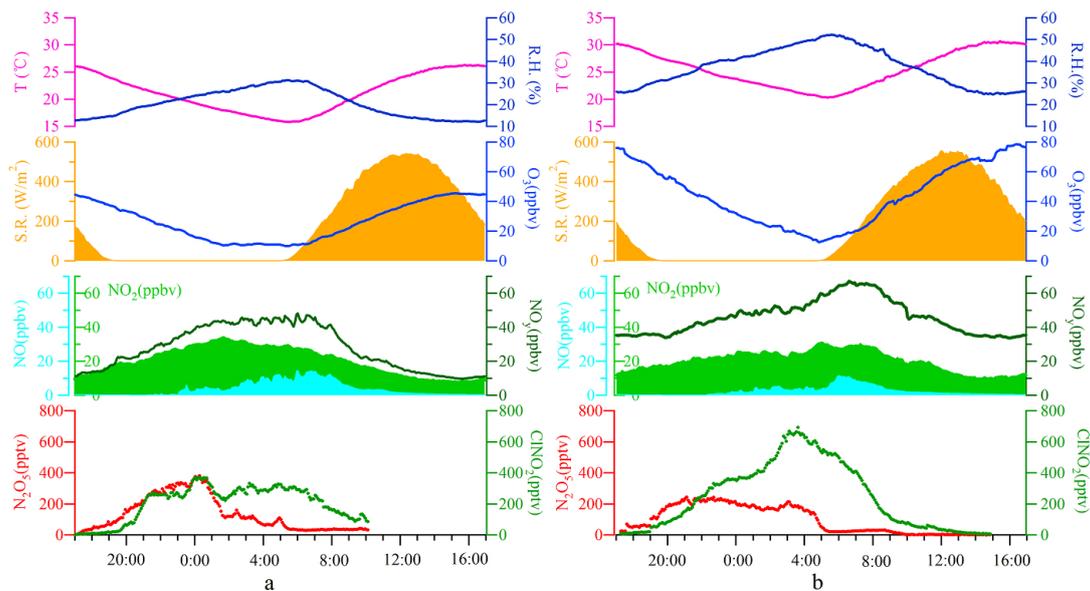


Figure S4: Two examples of the selected cases for deriving $\gamma(N_2O_5)$: **(a)** the night of May 20th; **(b)** the night of May 27th.

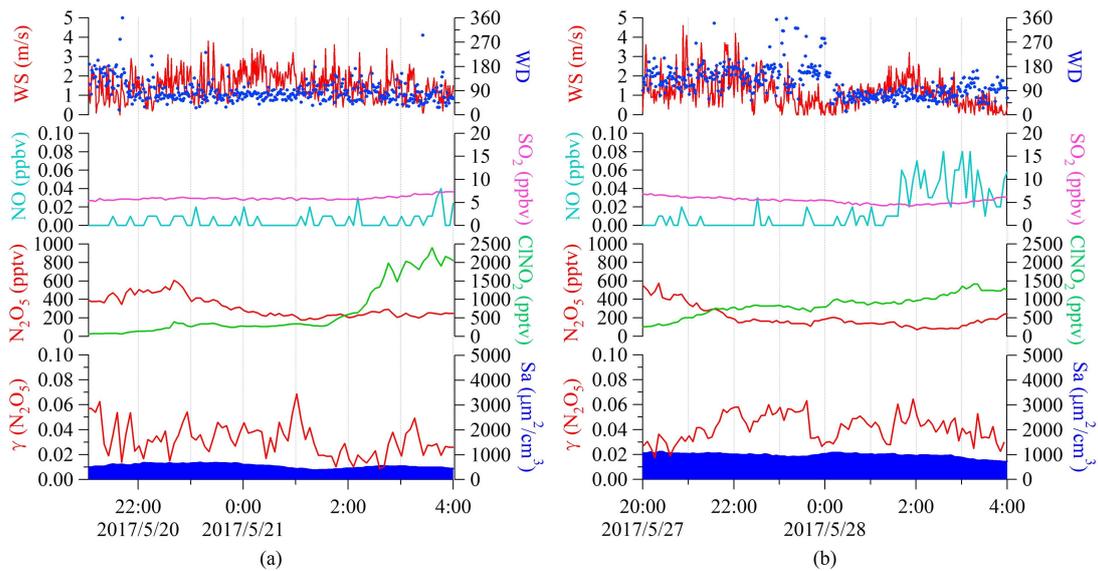


Figure S5. Relationship of $\gamma(\text{N}_2\text{O}_5)$ with aerosol water content ($[\text{H}_2\text{O}]$). The orange dots were derived on May 5th 23:00~05:00 which represent N_2O_5 uptake on sand dust particles. The blue dots denote $\gamma(\text{N}_2\text{O}_5)$ in the category of “urban air masses” (see Table 1 in the main text).

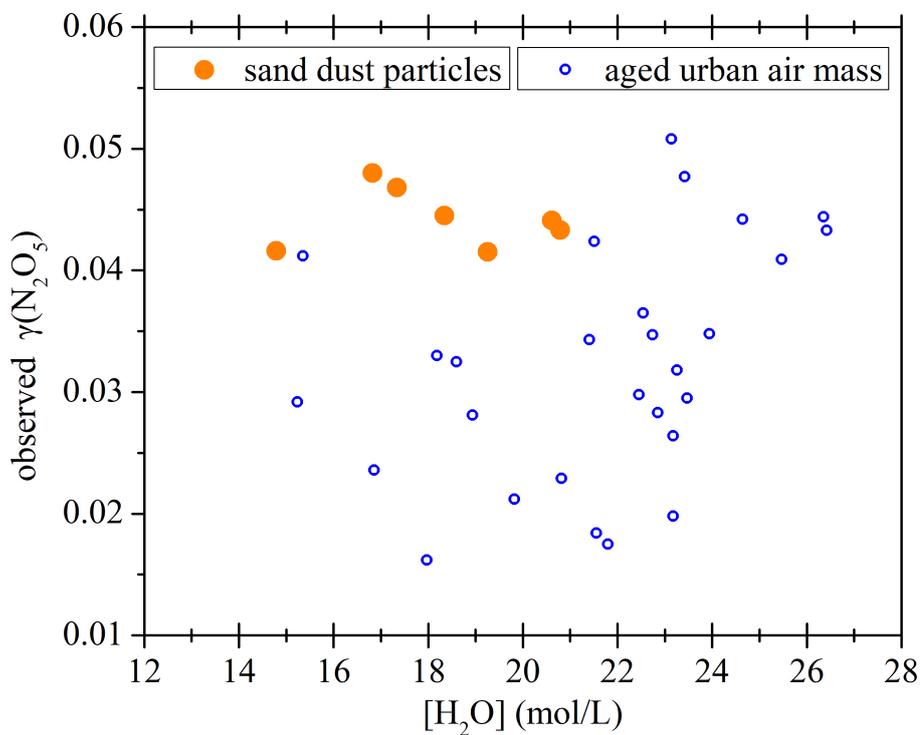


Figure S6: The relationship between $\text{PM}_{2.5}$ and S_a during the non-dust period (a), i.e., data during the sand storm event (May 4th to May 5th) was excluded from the plot. Since the dependence of S_a on $\text{PM}_{2.5}$ was found RH-dependent, we selected data in non-dust periods with

the same RH range of the sand storm event (29~36 %) and displayed the PM_{2.5}-S_a relationship in (b). The regression function was used to estimate the S_a in the sand storm event.

