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Supplement of

Modeling atmospheric mineral aerosol chemistry to predict heterogeneous photooxidation of SO₂

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Section 1: Chamber Characterization

The outdoor experiments were conducted using the University of Florida Atmospheric Photochemical Outdoor Reactor (UF–APHOR) dual chambers located on the roof of Black Hall at University of Florida, Gainesville, Florida (latitude/longitude: 29.64185°/-82.347883°). The total volume for the two half-cylinder shaped chamber is 52 m³ each. The surface to volume ratio is 1.65 m² m⁻³ for each chamber. The chambers are built with 0.13 mm FEP Teflon film. The meteorological parameters (i.e., temperature, relative humidity, sunlight spectrum and sunlight intensity) are monitored simultaneously both inside and outside the chambers using a hygrometer (CR1000 Measurement and Control System, Campbell Scientific) (temperature and humidity), a fibro-optical portable spectrometer (EPP2000, Stellar Net Inc., USA) (sunlight spectrum) and an ultraviolet radiometer (TUVR, Eppley Laboratory Inc.) (sunlight intensity). In addition, the wall loss rate constants of ozone, SO₂, H₂O₂ and HONO were measured via separate experiments. The rate constant of particle loss to the chamber wall was also measured for Arizona Test Dust (ATD) particles as well as the ammonia sulfate inorganic seeded aerosol. The particle loss rate was calculated for every 3 minutes within each particle size bin and then integrated to calculate an average particle loss rate. The typical particle distribution of ATD particles is shown in the Fig. S1.

Indoor chamber experiment

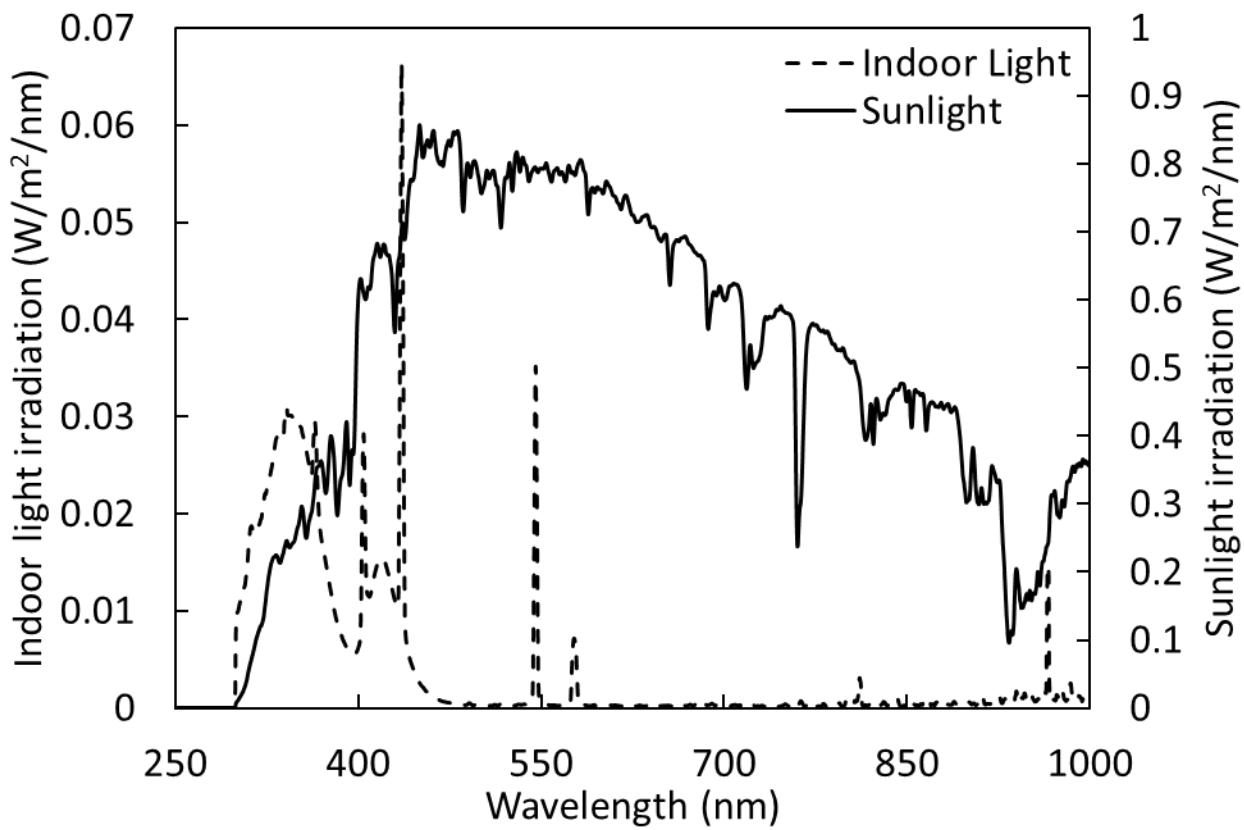
The indoor chamber experiments were performed in a 2 m³ Teflon indoor chamber equipped with UV lamps (Wavelength: 280nm – 900 nm) (Solarc Systems Inc., FS40T12/UVB). The RH and the concentration of trace gases and dust particles were controlled to variety specific experimental conditions. During the experiment, the gases were continuously measured directly from the indoor chamber using a gas chromatography–flame ionization detector (HP–5890 GC–FID), a fluorescence TRS analyzer (Teledyne Model 102E), and a chemiluminescence NO/NO_x analyzer (Teledyne Model T201). The suspend particles were continuously measured by a scanning mobility particle sizer (SMPS, TSI 3080, USA) and an Optical Particle Counter (OPC, TSI 3330, USA). The mass concentration of inorganic iron was measured using a Particle–Into–Liquid Sampler (Applikon, ADISO 2081) combined with Ion Chromatography (Metrohm, 761 Compact IC) (PILS–IC) for every 30 minutes.

Outdoor chamber experiment

The dual chambers were flushed and cleaned by the air purifier system (GC Series, IQ Air Inc.) for 2 days before each experiment. The background sulfate concentration was measured every time

before experiments. Non-reactive CCL₄ (400 ppb) was injected into the dual chamber to determine the chamber dilution factor. Due to the chamber dilution, ambient trace gases (i.e., CO, O₃, CH₄, HCHO and volatile organic compounds) outside the chamber are intruded into the chamber. The estimated concentration of background gases are 1.8 ppb CH₄, 18 ppb HCHO, 6 ppb CH₃CHO, 0.1 ppb isoprene
5 and 1 ppb HONO. The measurement procedures of gases and inorganic iron concentration were similar to that of indoor chamber experiments. The particle distribution was measured using the SMPS and the OPC. For measuring the total particle mass concentration, the suspended particles were collected on a 13mm diameter Teflon-coated glass fiber filter (Pall Life Science Pallflex, TX40HI20-WW) for 20 minutes. The filter mass difference was measured using a microbalance (MX5, Mettler Toledo,
10 Columbus, OH). The temperature (T, K) and relative humidity (RH, %) in the dual chamber were monitored using a hygrometer (CR1000 Measurement and Control System, Campbell Scientific). For measuring the wavelength-dependent actinic flux, a fibro-optical portable spectrometer (EPP2000, Stellar Net Inc., USA) and an ultraviolet radiometer (TUVR, Eppley Laboratory Inc.) were used.

Figure S1



5 Figure S1. Light irradiation of the indoor–UV light and the sunlight measured with a fibro-optical portable spectrometer (EPP2000, Stellar Net Inc., USA). The sunlight irradiance was measured on April 20th, 2016 in University of Florida Atmospheric Photochemical Outdoor Reactor, Florida, USA (latitude/longitude: $29.64185^\circ/-82.347883^\circ$).

Figure S2

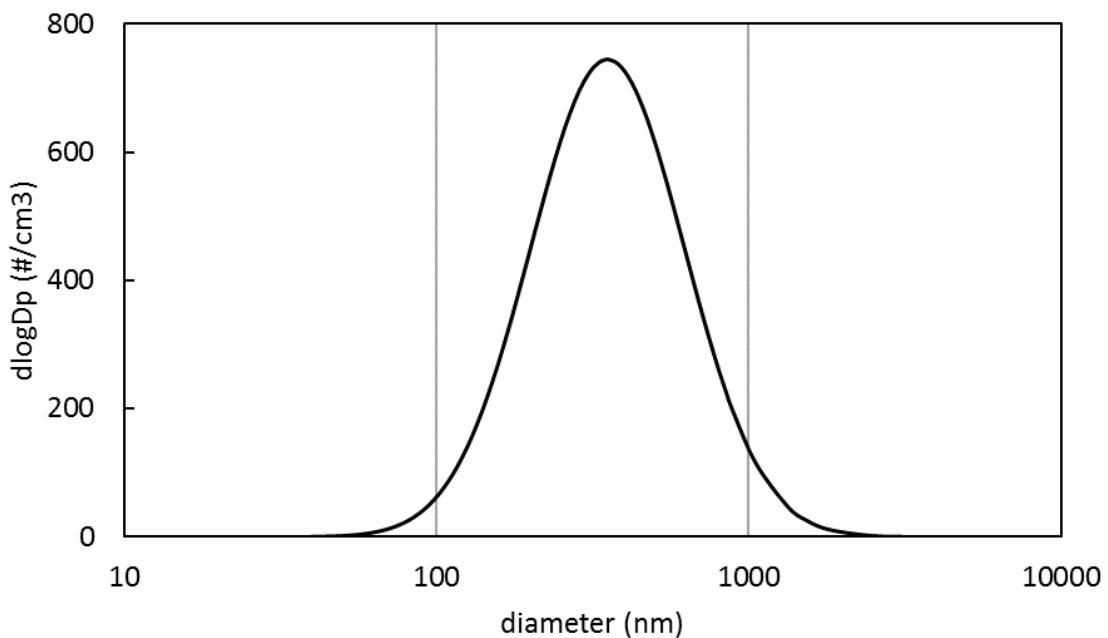


Figure S2. Typical particle size distribution of Arizona Test Dust particles for dust concentration of $74 \mu\text{g m}^{-3}$ for the experiment on June 16, 2015. The particle number concentration was measured
5 by combining a scanning mobility particle sizer (SMPS, TSI 3080, USA) and an Optical Particle Counter (OPC, TSI 3330, USA) using a Multi-instrument Manager (MIM2TM) Software provided by TSI.

Figure S3

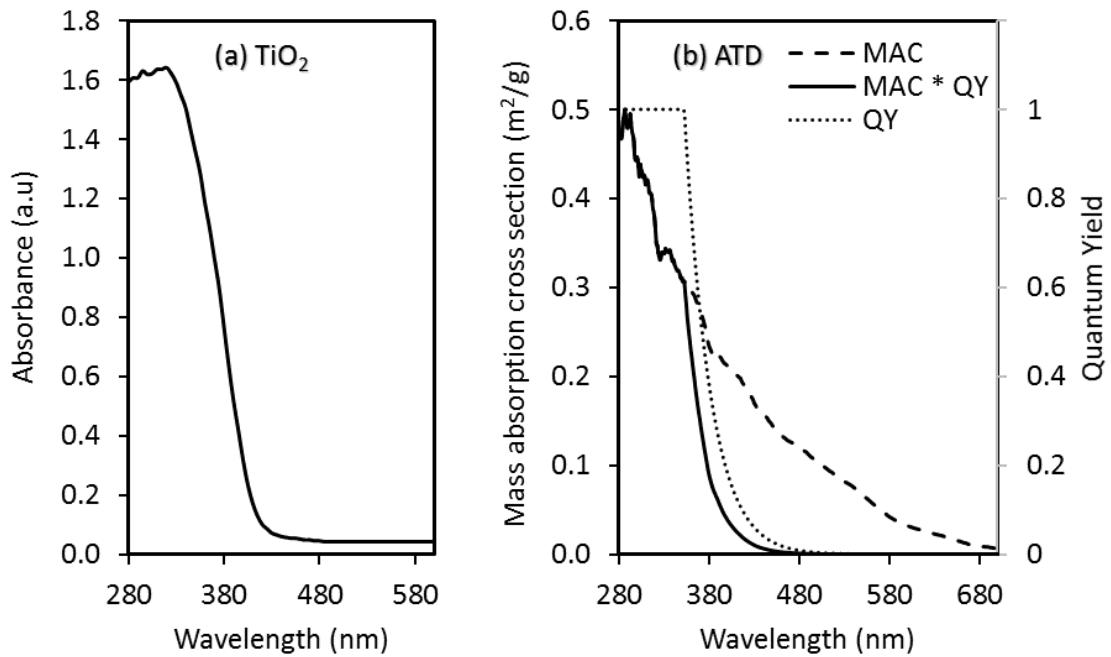


Figure S3. (a) Light absorption of TiO_2 (Reyes–Coronado et al., 2008) (b) The mass absorption cross section (MAC) and the quantum yield (QY) of Arizona Test Dust particles were multiplied
5 to calculate the photocatalytic rate coefficient. The quantum yield of Arizona Test Dust particles was derived from the absorption spectrum of TiO_2 .

Figure S4

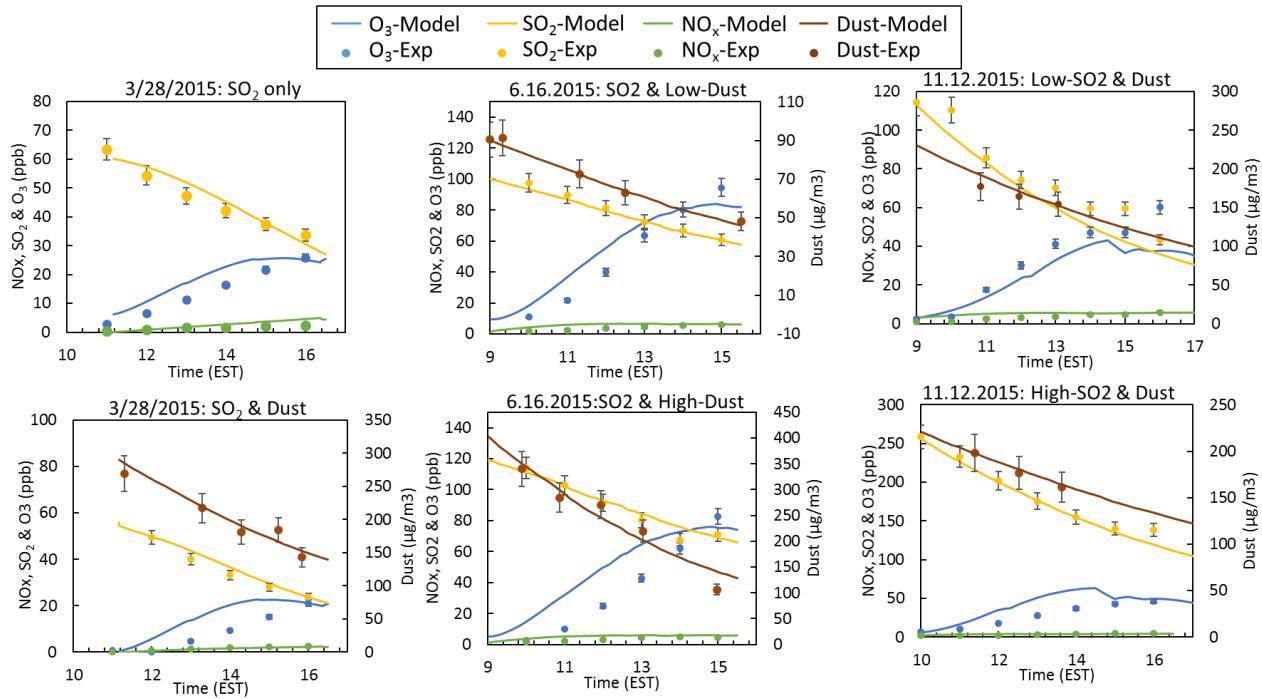


Figure S4. Simulated Ozone, NO_x, SO₂, and Dust concentration compare to outdoor experimental observation for Outdoor experiment (3/28/2015, 6/16/2015 and 11/12/2015). “Exp”

denotes the experimentally observation and “Model” denotes the model-predicted concentration of trace gases as well as ATD particles. All the simulations included the chamber dilution and the wall process of gaseous compounds and particles. The errors associated with the observation of SO₂, NO_x, O₃ and dust particle mass concentration were ±0.9%, ±12.5%, ±0.2% and ±6%, respectively.

Figure S5

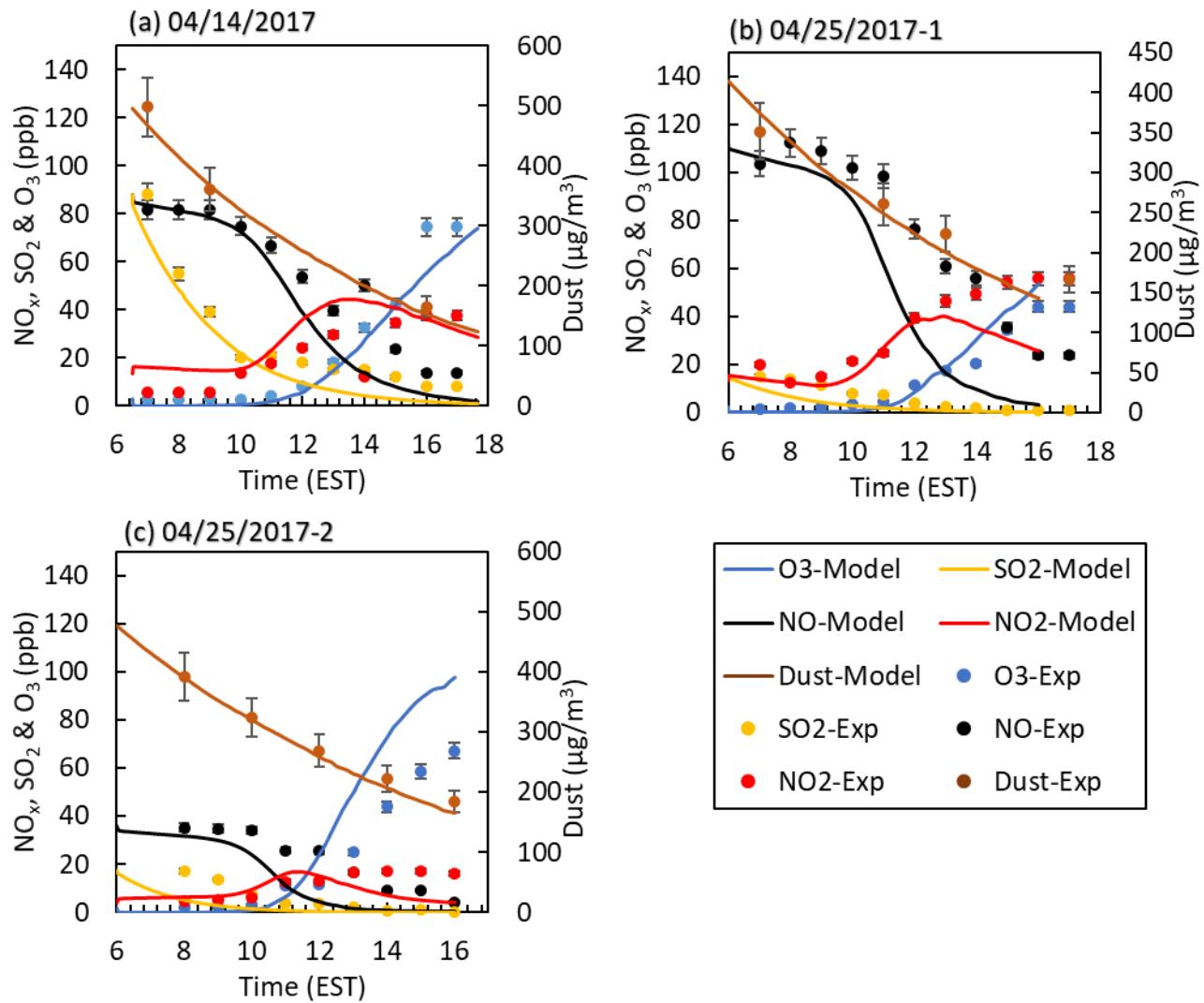
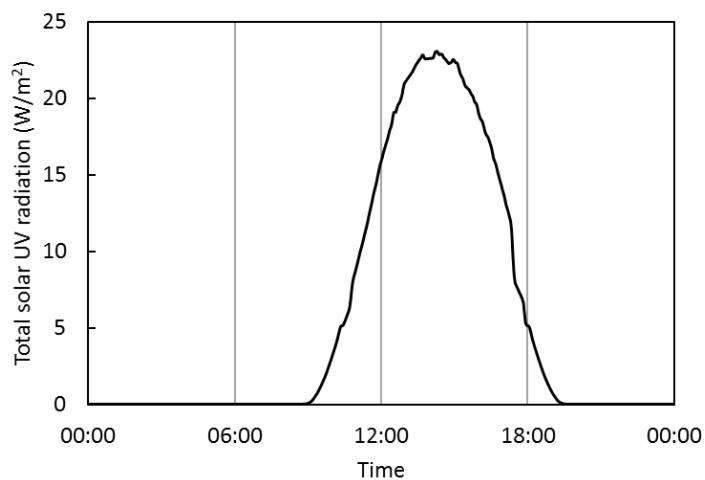


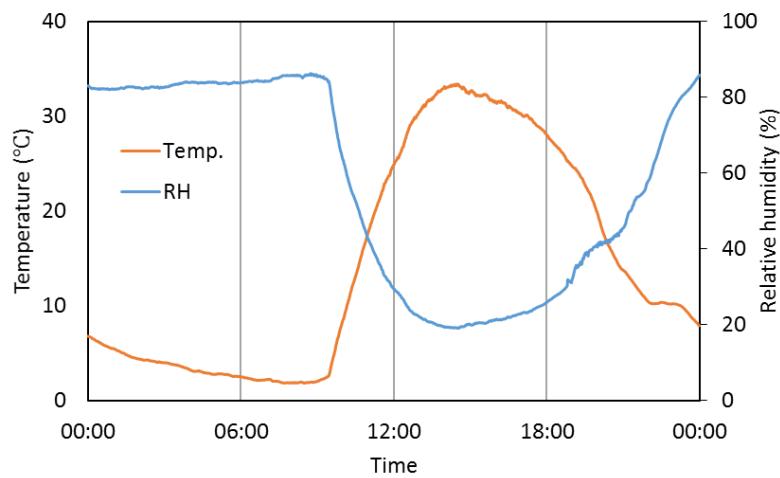
Figure S5. Simulated Ozone, NO_x , SO_2 , and Dust concentration compare to outdoor experimental observation for Outdoor experiment (4/14/2017 and 4/25/2017). “Exp” denotes the experimentally observation and “Model” denotes the model-predicted concentration of trace gases and ATD particles. All the simulations included the chamber dilution and the wall process of gaseous compounds and particles. The errors associated with the observation of SO_2 , NO , NO_2 , O_3 and dust particle mass concentration were $\pm 0.9\%$, $\pm 12.5\%$, $\pm 6.9\%$, $\pm 0.2\%$ and $\pm 6\%$, respectively.

Figure S6

(a) Total solar UV radiation



(b) Temperature and humidity



5

Figure S6. Time profile of (a) total solar UV irradiation and (b) temperature and humidity measured on November 12, 2015 at University of Florida Atmospheric Photochemical Outdoor Reactor, Florida, USA (latitude/longitude: 29.64185°/–82.347883°). The total solar short-wave radiation (0.295 to 0.385 μm) was measured using an ultraviolet radiometer (TUVR, Eppley 10 Laboratory Inc.) inside the chamber. The temperature and humidity are continuously monitored inside the chamber using a hygrometer (CR1000 Measurement and Control System, Campbell Scientific)

Figure S7

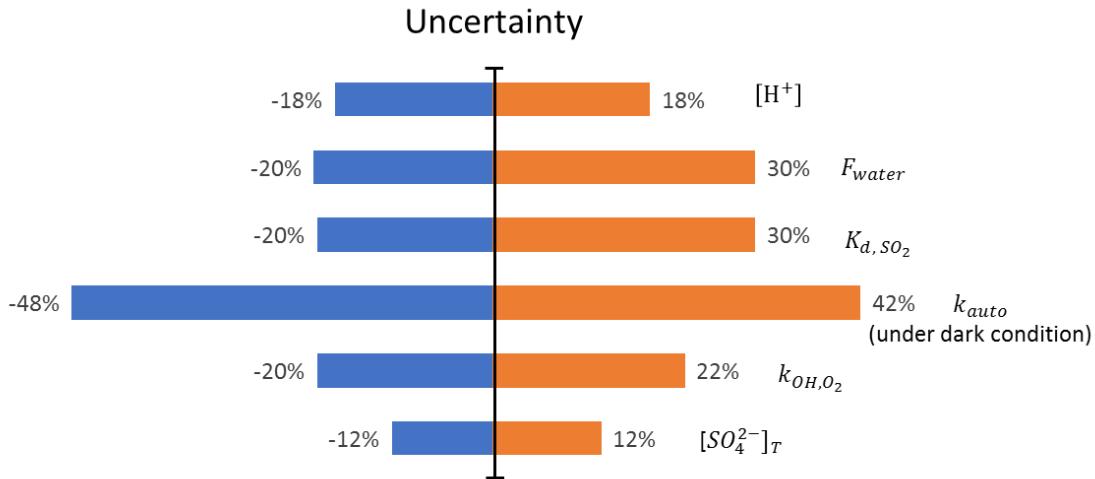
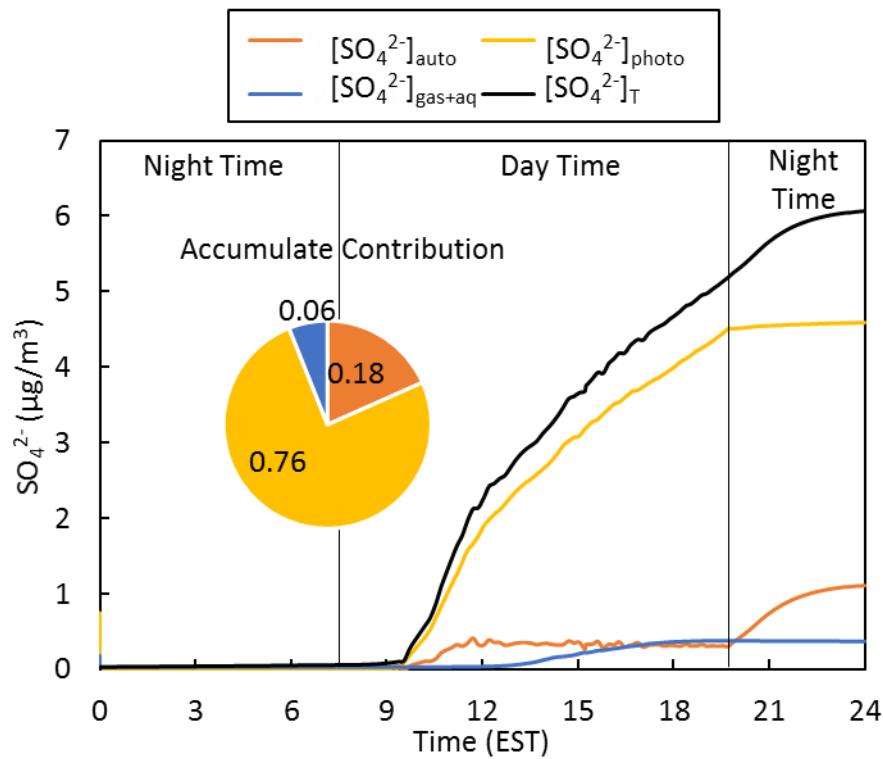


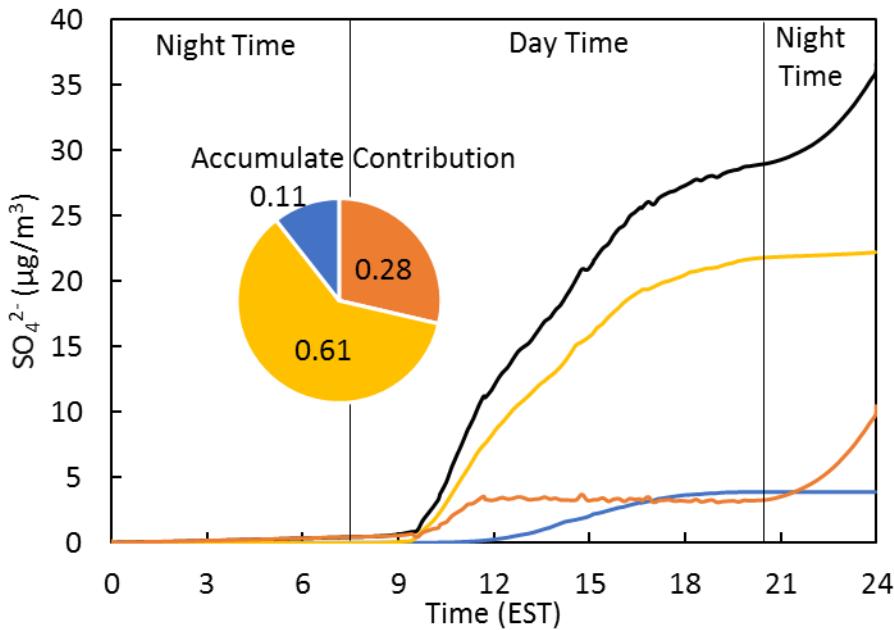
Figure S7. The uncertainty of major model parameters to predicted total sulfate. $[H^+]$ is estimated by E-AIM II (Clegg et al., 1998; Wexler and Clegg, 2002; Clegg and Wexler, 2011) and corrected for the ammonia rich condition (Li and Jang, 2012; Li et al., 2015). The reported uncertainty of $[H^+]$ associated with C–RUV technique is $\pm 18\%$. The uncertainty of F_{water} (coefficient of water to dry dust ratio in mass) is -20% to 30% due to the uncertainty of the measurement of sulfate and ammonium ions ($\pm 10\%$ each). The uncertainty of K_{d, so_2} (-20% to 30%) is calculated based on the uncertainty of $[H^+]$ and F_{water} using the propagation error (Eqs. (6) and (7)). The uncertainty of k_{auto} is estimated by simulating the formation of sulfate within the uncertainty in K_{d, so_2} (-20% to 30%) and the measurement of sulfate using PILS-IC ($\pm 10\%$) under dark condition. The uncertainty of k_{OHO_2} is estimated using the same approach to k_{auto} under ambient sunlight. The uncertainty of the prediction of sulfate ($[SO_4^{2-}]_T$) is estimated at the end of the simulation. The chamber simulation for the prediction of $[SO_4^{2-}]_T$ is conducted with 100 ppb of initial SO_2 , 2 ppb of initial NO_2 , 2 ppb of initial O_3 and $200 \mu g m^{-3}$ of ATD particles at $T = 298K$ and $RH = 40\%$ from 6 a.m. to 5 p.m based on the sunlight profile of April 25, 2017. NO_x (rate of flux = $2.7 \times 10^6, s^{-1}$) and isoprene ($2.7 \times 10^6, s^{-1}$) were constantly added to chamber for the dilution effects. The simulation was performed without considering the particle loss to the chamber wall.

Figure S8

(a) Rural area



5 (b) Urban area



- Figure S8. 24 hours simulation of attribution of sulfate formation under the rural (Fig. S8(a)) and polluted urban environment (Fig. S8(b)) using AMAR model. The total sulfate is simulated to show the composition including the sulfate formed from non-dust chemistry ($[\text{SO}_4^{2-}]_{\text{aq}} + [\text{SO}_4^{2-}]_{\text{gas}}$), from dust-phase autoxidation ($[\text{SO}_4^{2-}]_{\text{auto}}$), and from dust photochemistry ($[\text{SO}_4^{2-}]_{\text{photo}}$). The meteorological parameters (i.e., temperature and humidity) are obtained from outdoor chamber experiment (April 25, 2017, Table 2). The particle loss to the chamber wall was not considered into the simulation while the dilution process was included.
- In Fig. S8(a), 200 $\mu\text{g m}^{-3}$ of ATD particles, 2 ppb of initial SO_2 , 5 ppb of NO_x and 20 ppb of isoprene were set for the simulation of rural condition.
- In Fig. S8(b), 200 $\mu\text{g m}^{-3}$ of ATD particles, 30 ppb of initial SO_2 , 40 ppb of NO_x and 30 ppb of isoprene were set for the simulation of polluted condition.

Table S1. Chemical mechanism for AMAR model

Reaction	Rate constant ^a gas phase ^b	Note
1 $O^3P + SO_2 \rightarrow SO_3$	$9.75 \times 10^{-13} \exp(-2280/T)$	Baulch et al., 1984; Kerr, 1984
2 $HO_2 + SO_2 \rightarrow SO_3 + OH \cdot$	1.00×10^{-18}	Atkinson et al., 1989; Atkinson and Lloyd, 1984
3 $CH_3-O_2 \cdot + SO_2 \rightarrow SO_3 + CH_3-O \cdot$	5.00×10^{-17}	Atkinson et al., 1989; Atkinson and Lloyd, 1984
4 $CH_3-O \cdot + SO_2 \rightarrow CH_3-O-SO_2 \cdot$	5.50×10^{-13}	Calvert, 1983
5 $CH_3 \cdot + SO_2 \rightarrow CH_3(O)S(O) \cdot$	2.90×10^{-13}	Graedel, 1977
6 $SO_2 + h\nu \rightarrow SO_2^*$	$2 \times j[NO_2_to_O^3P]$	Graedel, 1977
7 $OH \cdot + SO_2 \rightarrow HOSO_2$	$9.07 \times 10^{-13} \exp(231/T)$	Atkinson et al., 1989; Kerr, 1984
8 $NO_2 + SO_2 \rightarrow NO + SO_3$	2.00×10^{-26}	Sander, 2006
9 $NO_3 + SO_2 \rightarrow NO_2 + SO_3$	7.00×10^{-21}	Sander, 2006
10 $CH_3-SO_3 \cdot \rightarrow SO_3 + CH_3 \cdot$	4.00×10^{-2}	Chen and Jang, 2012
11 $CH_3-SO_3 \cdot + H-CO-H \rightarrow CH_3-SO_3H + HO_2 \cdot + CO$	1.60×10^{-15}	Yin et al., 1990
12 $CH_3-SO_3 \cdot + HO_2 \rightarrow CH_3-SO_3H + O_2$	5.00×10^{-11}	Yin et al., 1990
13 $CH_3-SO_3 \cdot + HONO \rightarrow CH_3-SO_3H + NO_2$	6.60×10^{-16}	Yin et al., 1990
14 $CH_3-SO_3 \cdot + H_2O_2 \rightarrow CH_3-SO_3H + HO_2 \cdot$	3.00×10^{-16}	Yin et al., 1990
15 $CH_3-SO_3 \cdot + CH_3-OOH \rightarrow CH_3-SO_3H + CH_3-O_2 \cdot$	3.00×10^{-16}	Yin et al., 1990
16 $CH_3-SO_3 \cdot + CH_3-OH \rightarrow CH_3-SO_3H + H-CO-H + HO_2 \cdot$	1.00×10^{-16}	Yin et al., 1990
17 $CH_3-SO_3 \cdot + NO_2 \rightarrow CH_3(O)S(O)ONO_2$	3.00×10^{-15}	Yin et al., 1990
18 $CH_3(O)S(O)ONO_2 + H_2O \rightarrow CH_3-SO_3H + HNO_3$	1.00×10^{-15}	Yin et al., 1990
19 $CH_3-SO_3 \cdot + NO \rightarrow CH_3(O)S(O)ONO$	3.00×10^{-15}	Yin et al., 1990
20 $CH_3(O)S(O)ONO + H_2O \rightarrow CH_3-SO_3H + HONO$	1.00×10^{-15}	Yin et al., 1990
21 $CH_3(O)S(O) \cdot + NO_2 \rightarrow CH_3-SO_3 \cdot + NO$	5.00×10^{-13}	Chen and Jang, 2012
22 $CH_3(O)S(O) \cdot O_3 \rightarrow CH_3-SO_3 \cdot + O_2$	5.00×10^{-15}	Yin et al., 1990

Table S1. (continued)

Reaction	Rate constant ^a	Note
23 $\text{CH}_3(\text{O})\text{S}(\text{O}) \cdot + \text{HO}_2 \rightarrow \text{CH}_3-\text{SO}_3 \cdot + \text{OH}$	2.50×10^{-13}	Yin et al., 1990
24 $\text{CH}_3(\text{O})\text{S}(\text{O}) \cdot \rightarrow \text{CH}_3 \cdot + \text{SO}_2$	1.00×10^1	Mellouki et al., 1988
25 $\text{CH}_3(\text{O})\text{S}(\text{O}) \cdot + \text{O}_2 \rightarrow \text{CH}_3(\text{O})\text{S}(\text{O})\text{OO} \cdot$	2.60×10^{-18}	Yin et al., 1990
26 $\text{CH}_3(\text{O})\text{S}(\text{O})\text{OO} \cdot \rightarrow \text{CH}_3(\text{O})\text{S}(\text{O}) \cdot + \text{O}_2$	3.30	Yin et al., 1990
27 $\text{CH}_3(\text{O})\text{S}(\text{O}) \cdot + \text{NO}_3 \rightarrow \text{CH}_3-\text{SO} \cdot + \text{NO}_2$	1.00×10^{-14}	Yin et al., 1990
28 $\text{CH}_3(\text{O})\text{S}(\text{O}) \cdot + \text{CH}_3-\text{O}_2 \cdot \rightarrow \text{CH}_3-\text{SO}_3 \cdot + \text{CH}_3-\text{O} \cdot$	2.50×10^{-13}	Yin et al., 1990
29 $\text{CH}_3(\text{O})\text{S}(\text{O}) \cdot + \text{CH}_3-\text{S} \rightarrow \text{CH}_3(\text{O})\text{S}(\text{O})\text{S}-\text{CH}_3$	4.20×10^{-11}	Yin et al., 1990
30 $\text{CH}_3(\text{O})\text{S}(\text{O}) \cdot + \text{CH}_3(\text{O})\text{S}(\text{O}) \rightarrow \text{CH}_3-\text{SO} \cdot + \text{CH}_3-\text{SO}_3 \cdot$	7.50×10^{-12}	Yin et al., 1990
31 $\text{CH}_3(\text{O})\text{S}(\text{O}) \cdot + \text{CH}_3-\text{S}-\text{NO} \rightarrow \text{CH}_3(\text{O})\text{S}(\text{O})\text{CH}_3 + \text{NO}$	6.80×10^{-13}	Yin et al., 1990
32 $\text{CH}_3(\text{O})\text{S}(\text{O}) \cdot + \text{OH} \rightarrow \text{CH}_3-\text{SO}_3\text{H}$	5.00×10^{-11}	Yin et al., 1990
33 $\text{CH}_3(\text{O})\text{S}(\text{O})\text{OO} \cdot + \text{NO} \rightarrow \text{CH}_3-\text{SO}_3 \cdot + \text{NO}_2$	1.00×10^{-11}	Yin et al., 1990
34 $\text{CH}_3(\text{O})\text{S}(\text{O})\text{OO} \cdot + \text{NO}_2 \rightarrow \text{CH}_3(\text{O})\text{S}(\text{O})\text{OOONO}_2$	1.00×10^{-12}	Yin et al., 1990
35 $\text{CH}_3(\text{O})\text{S}(\text{O})\text{OOONO}_2 \rightarrow \text{CH}_3(\text{O})\text{S}(\text{O})\text{OO} \cdot + \text{NO}_2$	4.20×10^{-03}	Yin et al., 1990
36 $\text{CH}_3(\text{O})\text{S}(\text{O})\text{OO} \cdot + \text{CH}_3-\text{S} \rightarrow \text{CH}_3-\text{SO}_3 \cdot + \text{CH}_3-\text{SO} \cdot$	6.00×10^{-11}	Yin et al., 1990
37 $\text{CH}_3(\text{O})\text{S}(\text{O})\text{OO} \cdot + \text{CH}_3-\text{SO} \rightarrow \text{CH}_3-\text{SO}_3 \cdot + \text{CH}_3(\text{O})\text{S}(\text{O}) \cdot$	8.00×10^{-12}	Yin et al., 1990
38 $\text{CH}_3(\text{O})\text{S}(\text{O})\text{OO} \cdot + \text{CH}_3(\text{O})\text{S}(\text{O}) \rightarrow 2\text{CH}_3-\text{SO}_3 \cdot$	3.00×10^{-13}	Yin et al., 1990
39 $\text{CH}_3(\text{O})\text{S}(\text{O})\text{OO} \cdot + \text{HO}_2 \rightarrow \text{CH}_3(\text{O})\text{S}(\text{O})\text{OOH} \cdot + \text{O}_2$	2.00×10^{-12}	Yin et al., 1990
40 $\text{CH}_3(\text{O})\text{S}(\text{O})\text{OO} \cdot + \text{CH}_3-\text{O}_2 \rightarrow \text{CH}_3-\text{SO}_3 \cdot + \text{CH}_3-\text{O} \cdot + \text{O}_2$	5.50×10^{-12}	Yin et al., 1990
41 $\text{CH}_3(\text{O})\text{S}(\text{O})\text{OO} \cdot + \text{CH}_3(\text{O})\text{S}(\text{O})\text{OO} \cdot + \text{CH}_3-\text{SO} \rightarrow 2\text{CH}_3-\text{SO}_3 \cdot + \text{O}_2$	6.00×10^{-12}	Yin et al., 1990
42 $\text{CH}_3(\text{O})\text{S}(\text{O})\text{OO} \cdot + \text{CH}_3-\text{S}-\text{OH} \rightarrow \text{CH}_3(\text{O})\text{S}(\text{O})\text{OOH} + \text{CH}_3-\text{SO} \cdot$	4.00×10^{-13}	Yin et al., 1990
43 $\text{CH}_3-\text{SO} \cdot + \text{O}_2 \rightarrow \text{CH}_3-\text{S}(\text{O})\text{OO} \cdot$	7.70×10^{-18}	Yin et al., 1990
44 $\text{CH}_3-\text{S}(\text{O})\text{OO} \cdot \rightarrow \text{CH}_3-\text{SO} \cdot + \text{O}_2$	1.70×10^2	Yin et al., 1990
45 $\text{CH}_3-\text{SO} \cdot + \text{NO}_2 \rightarrow \text{CH}_3(\text{O})\text{S}(\text{O}) \cdot + \text{NO}$	6.00×10^{-12}	MCM v3.3
46 $\text{CH}_3-\text{SO} \cdot + \text{NO}_2 \rightarrow \text{CH}_3 \cdot + \text{NO} + \text{SO}_2$	3.00×10^{-12}	MCM v3.3
47 $\text{CH}_3-\text{SO} \cdot \rightarrow \text{SO} \cdot + \text{CH}_3 \cdot$	$2.66 \times 10^{32} \exp(-25200/T)$	Yin et al., 1990
48 $\text{CH}_3-\text{SO} \cdot + \text{NO}_3 \rightarrow \text{CH}_3(\text{O})\text{S}(\text{O}) \cdot + \text{NO}_2$	8.00×10^{-12}	Yin et al., 1990
49 $\text{CH}_3-\text{SO} \cdot + \text{O}_3 \rightarrow \text{CH}_3(\text{O})\text{S}(\text{O}) \cdot + \text{O}_2$	1.00×10^{-12}	Tyndall and Ravishankara, 1989

Table S1. (continued)

Reaction	Rate constant ^a	Note
51 $\text{CH}_3\text{-SO}\cdot + \text{CH}_3\text{-SO} \rightarrow \text{CH}_3\text{-SO}\cdot + \text{CH}_3(\text{O})\text{S(O)}\cdot$	7.50×10^{-12}	Yin et al., 1990
50 $\text{CH}_3\text{-SO}\cdot + \text{HO}_2 \rightarrow \text{CH}_3(\text{O})\text{S(O)}\cdot + \text{OH}$	1.50×10^{-12}	Yin et al., 1990
52 $\text{CH}_3\text{-SO}\cdot + \text{CH}_3\text{-O}_2 \rightarrow \text{CH}_3(\text{O})\text{S(O)}\cdot + \text{CH}_3\text{-O}\cdot$	3.00×10^{-12}	Yin et al., 1990
53 $\text{CH}_3\text{-SO}\cdot + \text{CH}_3\text{-NO} \rightarrow \text{CH}_3\text{-S-(O)CH}_3\cdot + \text{NO}$	6.80×10^{-13}	Yin et al., 1990
54 $\text{CH}_3\text{-SO}\cdot + \text{OH} \rightarrow \text{CH}_3\text{-S(O)OH}$	5.00×10^{-11}	Yin et al., 1990
55 $\text{CH}_3\text{-SO}\cdot + \text{O}_3 \rightarrow \text{SO}_2 + \text{CH}_3\text{-O}_2$	3.20×10^{-13}	Borissenko et al., 2003
56 $\text{CH}_3\text{-S}\cdot + \text{O}_2 \rightarrow \text{CH}_3\text{-SOO}\cdot$	5.80×10^{-17}	Sander, 2006
57 $\text{CH}_3\text{-SOO}\cdot \rightarrow \text{CH}_3\text{-S}\cdot + \text{O}_2$	6.00×10^2	Yin et al., 1990
58 $\text{CH}_3\text{-S}\cdot + \text{O}_3 \rightarrow \text{CH}_3\text{-SO}\cdot + \text{O}_2$	5.70×10^{-12}	Domine et al., 1992
59 $\text{CH}_3\text{-S}\cdot + \text{NO}_2 \rightarrow \text{CH}_3\text{-S-NO}_2\cdot$	6.10×10^{-13}	Yin et al., 1990
60 $\text{CH}_3\text{-S}\cdot + \text{NO}_2 \rightarrow \text{CH}_3\text{-SO}\cdot + \text{NO}$	6.10×10^{-11}	Yin et al., 1990
61 $\text{CH}_3\text{-S}\cdot + \text{NO} \rightarrow \text{CH}_3\text{-S-NO}\cdot$	2.87×10^{-11}	Balla et al., 1986
62 $\text{CH}_3\text{-S}\cdot + \text{NO}_3 \rightarrow \text{CH}_3\text{-SO}\cdot \text{NO}_2$	6.40×10^{-11}	Yin et al., 1990
63 $\text{CH}_3\text{-S}\cdot + \text{HO}_2 \rightarrow \text{CH}_3\text{-SO}\cdot + \text{OH}$	3.00×10^{-11}	Yin et al., 1990
64 $\text{CH}_3\text{-S}\cdot + \text{CH}_3\text{-O}_2 \rightarrow \text{CH}_3\text{-SO}\cdot + \text{CH}_3\text{-O}\cdot$	6.10×10^{-11}	Yin et al., 1990
65 $\text{CH}_3\text{-S}\cdot + \text{CH}_3\text{-S} \rightarrow \text{CH}_3\text{-S-S-CH}_3$	4.15×10^{-11}	Graham et al., 1964
66 $\text{CH}_3\text{-S}\cdot + \text{CH}_3\text{-S-NO} \rightarrow \text{CH}_3\text{-S-S-CH}_3 + \text{NO}$	1.40×10^{-12}	Yin et al., 1990
67 $\text{CH}_3\text{-S}\cdot + \text{OH} \rightarrow \text{CH}_3\text{-S-OH}$	5.00×10^{-11}	Yin et al., 1990
68 $\text{CH}_3\text{-S-NO}\cdot + h\nu \rightarrow \text{CH}_3\text{-S}\cdot + \text{NO}$	$0.5 \times j[\text{NO}_2\text{_to_O}^3\text{P}]$	Yin et al., 1990
69 $\text{CH}_3\text{-S}\cdot + \text{O}_3 \rightarrow \text{SO}_2 + \text{CH}_3\text{-O}\cdot$	5.70×10^{-12}	Domine et al., 1992
70 $\text{CH}_3\text{-S}\cdot + \text{CH}_3\text{-S-CH}_3 + (\text{O}_2) \rightarrow \text{CH}_3 + \text{CH}_3\text{-S(O)CH}_3 + \text{SO}\cdot$	8.00×10^{-12}	Chen and Jang, 2012
71 $\text{CH}_3\text{-S(O)OH} + \text{OH}\cdot \rightarrow \text{CH}_3(\text{O})\text{S(O)}\cdot + \text{H}_2\text{O}$	1.16×10^{-10}	Kukui et al., 2003
72 $\text{CH}_3\text{-S(O)OH} + \text{CH}_3\text{-SO}_3\cdot \rightarrow \text{CH}_3(\text{O})\text{S(O)}\cdot + \text{CH}_3\text{-SO}_3\text{H}$	2.00×10^{-13}	Yin et al., 1990
73 $\text{CH}_3\text{-S(O)OH} + \text{CH}_3\text{-O} \rightarrow \text{CH}_3(\text{O})\text{S(O)}\cdot + \text{CH}_3\text{-OH}$	1.00×10^{-13}	Yin et al., 1990
74 $\text{CH}_3\text{-S(O)OH} + \text{O}^3\text{P} \rightarrow \text{CH}_3(\text{O})\text{S(O)}\cdot + \text{OH}\cdot$	1.00×10^{-13}	Yin et al., 1990
75 $\text{CH}_3\text{-S(O)OH} + \text{NO}_3 \rightarrow \text{CH}_3(\text{O})\text{S(O)}\cdot + \text{HNO}_3$	1.00×10^{-13}	Yin et al., 1990
76 $\text{CH}_3\text{-S(O)OH} + \text{HO}_2 \rightarrow \text{CH}_3(\text{O})\text{S(O)}\cdot + \text{H}_2\text{O}_2$	1.00×10^{-15}	Yin et al., 1990

Table S1. (continued)

Reaction	Rate constant ^a	Note
77 $\text{CH}_3\text{-S(O)OH} + \text{CH}_3\text{-O}_2 \cdot \rightarrow \text{CH}_3(\text{O})\text{S(O)} \cdot + \text{CH}_3\text{-OOH}$	1.00×10^{-15}	Yin et al., 1990
78 $\text{CH}_3\text{-S-S-CH}_3 + \text{OH} \cdot \rightarrow \text{CH}_3\text{-S-OH} + \text{CH}_3\text{-S} \cdot$	$5.59 \times 10^{-11} \exp(380/T)$	Atkinson et al., 1989
79 $\text{CH}_3\text{-S-S-CH}_3 + \text{O}^3\text{P} \rightarrow \text{CH}_3\text{-SO} \cdot + \text{CH}_3\text{-S} \cdot$	$5.62 \times 10^{-11} \exp(250/T)$	Atkinson et al., 1989; Cvetanovic et al., 1981; Nip et al., 1981
80 $\text{CH}_3\text{-S-S-CH}_3 + \text{NO}_3 \rightarrow \text{CH}_3\text{-S(ONO}_2\text{)S-CH}_3$	7.00×10^{-13}	Yin et al., 1990
81 $\text{CH}_3\text{-S(ONO}_2\text{)S-CH}_3 \rightarrow \text{CH}_3\text{-S(O)NO}_2 \cdot + \text{CH}_3\text{-S} \cdot$	1.00×10^2	Yin et al., 1990
82 $\text{CH}_3\text{-S-S-CH}_3 + h\nu \rightarrow 2\text{CH}_3\text{-S} \cdot$	$5.0 \times 10^{-3} \times j[\text{NO}_2\text{-to-O}^3\text{P}]$	Yin et al., 1990
83 $\text{CH}_3\text{-S(O)NO}_2 \cdot \rightarrow \text{CH}_3\text{-SO} \cdot + \text{NO}_2$	1.00	Yin et al., 1990
84 $\text{SO}_2^* \rightarrow \text{SO}_2$	3.70×10^6	Graedel, 1977
85 $\text{SO}_2^* + \text{SO}_2 \rightarrow \text{SO} + \text{SO}_3$	6.30×10^{-13}	Graedel, 1977
86 $\text{SO}_2^* + \text{CO} \rightarrow \text{SO} + \text{CO}_2$	1.10×10^{-14}	Graedel, 1977
87 $\text{HOSO}_2 + \text{O}_2 \rightarrow \text{HO}_2 + \text{SO}_3$	4.00×10^{-13}	Atkinson et al., 1989; Kerr, 1984
88 $\text{HOSO}_2 + \text{OH} \cdot + \text{M} \rightarrow \text{H}_2\text{SO}_4 + \text{M}$	1.00×10^{-11}	Graedel, 1979
89 $\text{SO}_3 + \text{H}_2\text{O} + \text{M} \rightarrow \text{H}_2\text{SO}_4 + \text{M}$	9.10×10^{-13}	Atkinson and Lloyd, 1984; Kerr, 1984
90 $\text{SO}_3 + \text{O}^3\text{P} \rightarrow \text{SO}_2 + \text{O}_2$	7.00×10^{-13}	Calvert et al., 1978
91 $\text{SO} \cdot + \text{O}_2 \rightarrow \text{SO}_2 + \text{O}^3\text{P} \cdot$	$1.39 \times 10^{-13} \exp(-2280/T)$	Atkinson et al., 1989
92 $\text{SO} \cdot + \text{NO}_2 \rightarrow \text{SO}_2 + \text{NO}$	1.40×10^{-11}	Atkinson et al., 1989
93 $\text{SO} \cdot + \text{O}_3 \rightarrow \text{SO}_2 + \text{O}_2$	$4.51 \times 10^{-12} \exp(-1170/T)$	Atkinson et al., 1989
94 $\text{SO} \cdot + \text{O}^3\text{P} \rightarrow \text{SO}_2$	2.20×10^{-11}	Graedel, 1977
95 $\text{SO} \cdot + \text{OH} \rightarrow \text{SO}_2 + \text{HO}_2$	1.10×10^{-10}	Graedel, 1977
96 $\text{SO} \cdot + \text{SO}_3 \rightarrow 2\text{SO}_2$	2.00×10^{-15}	Graedel, 1977
Aqueous phase ^c		
1 $\text{OH(aq)} + \text{HO}_2\text{(aq)} \rightarrow \text{H}_2\text{O(aq)} + \text{O}_2\text{(aq)}$	$1.01 \times 10^{12} \exp(-1500/T)/V$	Sehested et al., 1968; Thomas, 1963
2 $\text{OH(aq)} + \text{O}_2^- \rightarrow \text{O}_2\text{(aq)} + \text{OH}^-$	$1.30 \times 10^{12} \exp(-1500/T)/V$	Buxton et al., 1988
3 $\text{HO}_2\text{(aq)} + \text{O}_2^- \rightarrow \text{H}_2\text{O}_2\text{(aq)} + \text{O}_2\text{(aq)} + \text{OH}^-$	$3.29 \times 10^9 \exp(-1050/T)/V$	Bielski et al., 1985

Table S1. (continued)

Reaction	Rate constant ^a	Note
4 $\text{HO}_2(\text{aq}) + \text{HO}_2(\text{aq}) \rightarrow \text{H}_2\text{O}_2(\text{aq}) + \text{O}_2(\text{aq})$	$7.14 \times 10^9 \exp(-2700/T)/\text{V}$	Bielski et al., 1985
5 $\text{OH}(\text{aq}) + \text{H}_2\text{O}_2(\text{aq}) \rightarrow \text{HO}_2(\text{aq}) + \text{H}_2\text{O}(\text{aq})$	$8.11 \times 10^9 \exp(-1700/T)/\text{V}$	Christensen et al., 1982; Buxton et al., 1988
6 $\text{O}_2^- + \text{O}_3(\text{aq}) \rightarrow \text{OH}(\text{aq}) + \text{OH}^- + 2\text{O}_2(\text{aq})$	$2.30 \times 10^{11} \exp(-1500/T)/\text{V}$	Sehested et al., 1983; Bielski et al., 1985;
7 $\text{H}_2\text{O}_2(\text{aq}) + h\nu \rightarrow \text{OH}(\text{aq}) + \text{OH}(\text{aq})$	$j[\text{H}_2\text{O}_2\text{_to_OH}]$	Lin et al., 1978; Molina et al., 1981; Nicovich et al., 1988; Vaghjiani et al., 1989
8 $\text{OH}(\text{aq}) + \text{HSO}_3^- \rightarrow \text{SO}_5^- + \text{H}_2\text{O}(\text{aq})$	$6.91 \times 10^{11} \exp(-1500/T)/\text{V}$	Huie and Neta, 1987
9 $\text{HSO}_3^- + \text{H}^+ + \text{H}_2\text{O}_2(\text{aq}) \rightarrow \text{SO}_4^{2-} + 2\text{H}^+$	$5.77 \times 10^{14} \exp(-4725/T)/\text{V}$	Hoffmann and Calvert, 1985
10 $\text{SO}_3^{2-} + \text{H}^+ + \text{H}_2\text{O}_2(\text{aq}) \rightarrow \text{SO}_4^{2-} + \text{H}^+$	$5.77 \times 10^{14} \exp(-4725/T)/\text{V}$	Hoffmann and Calvert, 1985
11 $\text{H}_2\text{C}(\text{OH})_2 + \text{OH}(\text{aq}) \rightarrow \text{HO}_2(\text{aq}) + \text{HCOOH}(\text{aq})$	$2.21 \times 10^{10} \exp(-1000/T)/\text{V}$	Chin and Wine, 1994
12 $\text{OH}(\text{aq}) + \text{SO}_3^{2-} \rightarrow \text{SO}_5^- + \text{OH}^-$	$8.44 \times 10^{11} \exp(-1500/T)/\text{V}$	Huie and Neta, 1987; Adams and Boag, 1964; Buxton et al., 1988
13 $\text{HCOO}^- + \text{OH}(\text{aq}) \rightarrow \text{CO}_2 + \text{HO}_2(\text{aq}) + \text{OH}^-$	$2.12 \times 10^{11} \exp(-1250/T)/\text{V}$	Chin and Wine, 1994
14 $\text{HSO}_3^- + \text{H}^+ + \text{CH}_3\text{OOH}(\text{aq}) \rightarrow \text{SO}_4^{2-} + 2\text{H}^+ + \text{CH}_3\text{OH}(\text{aq})$	$6.13 \times 10^{12} \exp(-3780/T)/\text{V}$	Hoffmann and Calvert, 1985
15 $\text{SO}_3^{2-} + \text{SO}_4^- \rightarrow \text{SO}_4^{2-} + \text{SO}_5^-$	$1.15 \times 10^{11} \exp(-1500/T)/\text{V}$	Wine et al., 1989
16 $\text{HSO}_3^- + \text{SO}_4^- \rightarrow \text{SO}_4^{2-} + \text{SO}_5^- + \text{H}^+$	$1.15 \times 10^{11} \exp(-1500/T)/\text{V}$	Wine et al., 1989
17 $\text{HSO}_3^- + \text{H}_2\text{C}(\text{OH})_2 \rightarrow \text{HOCH}_2\text{SO}_3^-$	$1.01 \times 10^4 \exp(-3000/T)/\text{V}$	Boyce and Hoffmann, 1984
18 $\text{SO}_3^{2-} + \text{H}_2\text{C}(\text{OH})_2 \rightarrow \text{HOCH}_2\text{SO}_3^- + \text{OH}^-$	$5.21 \times 10^7 \exp(-2450/T)/\text{V}$	Boyce and Hoffmann, 1984
19 $\text{HSO}_3^- + \text{O}_3(\text{aq}) \rightarrow \text{SO}_4^{2-} + \text{H}^+$	$3.83 \times 10^{13} \exp(-5500/T)/\text{V}$	Hoffmann and Calvert, 1985
20 $\text{SO}_3^{2-} + \text{O}_3(\text{aq}) \rightarrow \text{SO}_4^{2-}$	$7.43 \times 10^{16} \exp(-5280/T)/\text{V}$	Hoffmann and Calvert, 1985
21 $\text{SO}_4^- + \text{OH}^- \rightarrow \text{SO}_4^{2-} + \text{OH}(\text{aq})$	$1.23 \times 10^{10} \exp(-1500/T)/\text{V}$	Maruthamuthu and Neta, 1978
22 $\text{SO}_4^- + \text{H}_2\text{O}_2(\text{aq}) \rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{HO}_2(\text{aq})$	$9.86 \times 10^9 \exp(-2000/T)/\text{V}$	Wine et al., 1989
23 $\text{SO}_4^- + \text{H}_2\text{O}(\text{aq}) \rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{OH}(\text{aq})$	$2.19 \times 10^5 \exp(-1850/T)/\text{V}$	Bao and Barker, 1996
24 $\text{SO}_4^- \text{HCOO}^- \rightarrow \text{SO}_4^{2-} + \text{CO}_2(\text{aq}) + \text{OH}_2(\text{aq})$	$1.69 \times 10^{10} \exp(-1500/T)/\text{V}$	Wine et al., 1989
25 $\text{CH}_3\text{O}_2(\text{aq}) + \text{O}_2^- \rightarrow \text{CH}_3\text{OOH}(\text{aq}) + \text{OH}^- + \text{O}_2(\text{aq})$	$1.70 \times 10^9 \exp(-1050/T)/\text{V}$	Jacob, 1986

Table S1. (continued)

Reaction	Rate constant ^a	Note
26 $\text{HCOOH(aq)} + \text{OH(aq)} \rightarrow \text{H}_2\text{O(aq)} + \text{CO}_2(\text{aq}) + \text{HO}_2(\text{aq})$	$3.15 \times 10^9 \exp(-1000/T)/\text{V}$	Chin and Wine, 1994
27 $\text{O}_3(\text{aq}) + \text{H}_2\text{O}_2(\text{aq}) + \text{OH}^- \rightarrow \text{OH(aq)} + \text{O}_2^- + \text{O}_2(\text{aq}) + \text{H}_2\text{O(aq)}$	$2.97 \times 10^{14} \exp(-4000/T)/\text{V}$	Staehelin and Hoigne, 1982
28 $\text{HOCH}_2\text{SO}_3^- + \text{OH}^- \rightarrow \text{SO}_3^{2-} + \text{H}_2\text{C(OH)}_2$	$1.34 \times 10^{10} \exp(-4500/T)/\text{V}$	Deister et al., 1986; Munger et al., 1986
29 $\text{CH}_3\text{OOH(aq)} + \text{OH(aq)} \rightarrow \text{H}_2\text{C(OH)}_2(\text{aq}) + \text{OH(aq)}$	$9.44 \times 10^9 \exp(-1850/T)/\text{V}$	Jacob, 1986
30 $\text{CH}_3\text{OOH(aq)} + \text{OH(aq)} \rightarrow \text{CH}_3\text{O}_2(\text{aq}) + \text{H}_2\text{O(aq)}$	$8.11 \times 10^9 \exp(-1700/T)/\text{V}$	Jacob, 1986
31 $\text{HOCH}_2\text{SO}_3^- + \text{OH(aq)} \rightarrow \text{H}_2\text{C(OH)}_2(\text{aq}) + \text{SO}_5^- + \text{H}^+ + \text{OH}^-$	$2.00 \times 10^{11} \exp(-1500/T)/\text{V}$	Martin et al., 1989
32 $\text{SO}_4^- + \text{HO}_2(\text{aq}) \rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{O}_2(\text{aq})$	$7.67 \times 10^{11} \exp(-1500/T)/\text{V}$	Jacob, 1986
33 $\text{SO}_4^- + \text{O}_2^- \rightarrow \text{SO}_4^{2-} + \text{O}_2(\text{aq})$	$7.67 \times 10^{11} \exp(-1500/T)/\text{V}$	Jacob, 1986
34 $\text{HCOO}^- + \text{O}_3(\text{aq}) \rightarrow \text{CO}_2(\text{aq}) + \text{OH(aq)} + \text{O}_2^-$	$1.04 \times 10^{10} \exp(-5500/T)/\text{V}$	Hoigne and Bader, 1983
35 $\text{SO}_5^- + \text{HCOO}^- \rightarrow \text{HSO}_5^- + \text{CO}_2(\text{aq}) + \text{O}_2^-$	$9.45 \times 10^9 \exp(-4000/T)/\text{V}$	Jacob, 1986
36 $\text{SO}_4^- + \text{NO}_2^- \rightarrow \text{SO}_4^{2-} + \text{NO}_2(\text{aq})$	$1.50 \times 10^{11} \exp(-1500/T)/\text{V}$	Wine et al., 1989
37 $\text{SO}_5^- + \text{HSO}_3^- \rightarrow \text{HSO}_5^- + \text{SO}_5^-$	$1.02 \times 10^{10} \exp(-3850/T)/\text{V}$	Huie and Neta, 1987
38 $\text{HSO}_5^- + \text{OH(aq)} \rightarrow \text{SO}_5^- + \text{H}_2\text{O(aq)}$	$9.99 \times 10^9 \exp(-1900/T)/\text{V}$	Maruthamuthu and Neta, 1977
39 $\text{HSO}_5^- + \text{HSO}_3^- + \text{H}^+ \rightarrow 2\text{SO}_4^{2-} + 3\text{H}^+$	$1.40 \times 10^{10} \exp(-2000/T)/\text{V}$	McElroy, 1987; Betterton and Hoffmann, 1988a
40 $\text{SO}_5^- + \text{HSO}_3^- \rightarrow \text{SO}_4^- + \text{SO}_4^{2-} + \text{H}^+$	$9.46 \times 10^9 \exp(-3500/T)/\text{V}$	Huie and Neta, 1987
41 $\text{O}_2^- + \text{SO}_5^- \rightarrow \text{O}_2(\text{aq}) + \text{HSO}_5^- + \text{OH}^-$	$3.39 \times 10^9 \exp(-1050/T)/\text{V}$	Jacob, 1986
42 $\text{NO(aq)} + \text{NO}_2(\text{aq}) + \text{H}_2\text{O(aq)} \rightarrow 2\text{NO}_2^- + 2\text{H}^+$	$3.07 \times 10^{10} \exp(-1500/T)/\text{V}$	Lee, 1984
43 $\text{NO}_2(\text{aq}) + \text{NO}_2(\text{aq}) + \text{H}_2\text{O(aq)} \rightarrow \text{NO}_2^- + 2\text{H}^+ + \text{NO}_3^-$	$1.53 \times 10^{10} \exp(-1500/T)/\text{V}$	Lee, 1984
44 $\text{NO}_2(\text{aq}) + \text{OH(aq)} \rightarrow \text{NO}_3^- + \text{H}^+$	$2.00 \times 10^{11} \exp(-1500/T)/\text{V}$	Strehlow and Wagner, 1982
45 $\text{HONO(aq)} + h\nu \rightarrow \text{OH(aq)} + \text{NO(aq)}$	j[HONO_to_OH]	Bongartz et al., 1991; Atkinson et al., 1997
46 $\text{NO}_2^- + h\nu \rightarrow \text{OH(aq)} + \text{NO(aq)}$	j[HONO_to_OH]	Bongartz et al., 1991; Atkinson et al., 1997
47 $\text{HONO(aq)} + \text{OH(aq)} \rightarrow \text{NO}_2(\text{aq}) + \text{H}_2\text{O(aq)}$	$1.53 \times 10^{11} \exp(-1500/T)/\text{V}$	Rettich, 1978
48 $\text{NO}_2^- + \text{OH(aq)} \rightarrow \text{NO}_2(\text{aq}) + \text{OH}^-$	$1.53 \times 10^{12} \exp(-1500/T)/\text{V}$	Treinin and Hayon, 1970

Table S1. (continued)

Reaction	Rate constant ^a	Note
49 $\text{HONO}(\text{aq}) + \text{H}_2\text{O}_2(\text{aq}) + \text{H}^+ \rightarrow \text{NO}_3^- + \text{H}_2\text{O}(\text{aq}) + 2\text{H}^+$	$3.66 \times 10^{13} \exp(-6700/T)/\text{V}$	Lee and Lind, 1986
50 $\text{NO}_2^- + \text{O}_3(\text{aq}) \rightarrow \text{NO}_3^- + \text{O}_2(\text{aq})$	$6.72 \times 10^{15} \exp(-6950/T)/\text{V}$	Damschen and Martin, 1983
Gas-aqueous partitioning ^d		
1 $\text{SO}_2 \leftrightarrow \text{SO}_2(\text{aq})$	$2.66 \times 10^{-18} \exp(3135/T) \times T/(V(\text{aq})\rho_{\text{in}})$	Chameides, 1984
2 $\text{NO}_2 \leftrightarrow \text{NO}_2(\text{aq})$	$2.34 \times 10^{-18} \exp(1800/T) \times T/(V(\text{aq})\rho_{\text{in}})$	Chameides, 1984
3 $\text{NO} \leftrightarrow \text{NO}(\text{aq})$	$1.02 \times 10^{-18} \exp(1500/T) \times T/(V(\text{aq})\rho_{\text{in}})$	Schwartz and White, 1981
4 $\text{O}_3 \leftrightarrow \text{O}_3(\text{aq})$	$3.07 \times 10^{-19} \exp(2380/T) \times T/(V(\text{aq})\rho_{\text{in}})$	Chameides, 1984; Jacob, 1986
5 $\text{H}_2\text{O}_2 \leftrightarrow \text{H}_2\text{O}_2(\text{aq})$	$1.48 \times 10^{-18} \exp(6600/T) \times T/(V(\text{aq})\rho_{\text{in}})$	Chameides, 1984; O'Sullivan et al., 1996;
6 $\text{HONO} \leftrightarrow \text{HONO}(\text{aq})$	$4.80 \times 10^{-19} \exp(4750/T) \times T/(V(\text{aq})\rho_{\text{in}})$	Chameides, 1984; Martin, 1984
7 $\text{HO}_2 \leftrightarrow \text{HO}_2(\text{aq})$	$3.95 \times 10^{-20} \exp(6600/T) \times T/(V(\text{aq})\rho_{\text{in}})$	Hanson et al., 1992; Jacob, 1986
8 $\text{OH} \leftrightarrow \text{OH}(\text{aq})$	$4.58 \times 10^{-20} \exp(5250/T) \times T/(V(\text{aq})\rho_{\text{in}})$	Hanson et al., 1992; Jacob, 1986
9 $\text{CH}_3\text{O}_2 \leftrightarrow \text{CH}_3\text{O}_2(\text{aq})$	$3.39 \times 10^{-21} \exp(5600/T) \times T/(V(\text{aq})\rho_{\text{in}})$	Jacob, 1986
10 $\text{CH}_3\text{CO}_2\text{H} \leftrightarrow \text{CH}_3\text{CO}_2\text{H}(\text{aq})$	$3.40 \times 10^{-19} \exp(6400/T) \times T/(V(\text{aq})\rho_{\text{in}})$	Lind and Kok, 1986
11 $\text{HCHO} \leftrightarrow \text{HCHO}(\text{aq})$	$7.79 \times 10^{-24} \exp(7150/T) \times T/(V(\text{aq})\rho_{\text{in}})$	Chameides, 1984; Zhou and Mopper, 1990
12 $\text{CH}_3\text{OOH} \leftrightarrow \text{CH}_3\text{OOH}(\text{aq})$	$1.24 \times 10^{-19} \exp(5600/T) \times T/(V(\text{aq})\rho_{\text{in}})$	Lind and Kok, 1986
13 $\text{HCOOH} \leftrightarrow \text{HCOOH}(\text{aq})$	$1.46 \times 10^{-18} \exp(5700/T) \times T/(V(\text{aq})\rho_{\text{in}})$	Jacob, 1986
Acid dissociation		
1 $\text{HO}_2(\text{aq}) \leftrightarrow \text{O}_2^- + \text{H}^+$	$1.17 \times 10^{-3} \exp(-1046.4/T)$	Bielski et al., 1985
2 $\text{HCOOH}(\text{aq}) \leftrightarrow \text{HCOO}^- + \text{H}^+$	$1.79 \times 10^{-4} \exp(2.4/T)$	Sillen et al., 1964
3 $\text{HONO}(\text{aq}) \leftrightarrow \text{NO}_2^- + \text{H}^+$	$3.07 \times 10^{-4} \exp(151.6/T)$	Schwartz and White, 1981
4 $\text{SO}_2(\text{aq}) \leftrightarrow \text{HSO}_3^- + \text{H}^+$	$2.65 \times 10^{-2} \exp(-235.7/T)$	Olson and Hoffmann, 1989
5 $\text{HSO}_3^-(\text{aq}) \leftrightarrow \text{SO}_3^{2-} + \text{H}^+$	$1.21 \times 10^{-7} \exp(-180.4/T)$	Olson and Hoffmann, 1989
6 $\text{HCHO}(\text{aq}) \leftrightarrow \text{H}_2\text{C}(\text{OH})_2(\text{aq})$	$2.08 \times 10^2 \exp(-483.5/T)$	Betterton and Hoffmann, 1988b

Table S1. (continued)

Reaction	Rate constant ^a	k ₁	k ₂	k ₃	Note
Gas-dust partitioning ^e					
1 SO ₂ + Dust → SO ₂ (d) + Dust	f	1×10 ⁻⁸			Adams et al., 2005; Huang et al., 2015
2 SO ₂ (d) → SO ₂	g	1×10 ⁹	3100	0.013	Adams et al., 2005; Huang et al., 2015
3 O ₃ + Dust → O ₃ (d) + Dust	f	1×10 ⁻⁸			Michel et al. 2003; Underwood et al. 2001
4 O ₃ (d) → O ₃	g	3×10 ¹⁰	2700	0	Michel et al. 2003; Underwood et al. 2001
5 NO ₂ + Dust → NO ₂ (d) + Dust	f	1×10 ⁻⁸			Chameides 1984
6 NO ₂ (d) → NO ₂	g	1×10 ¹⁰	2500	0	Chameides 1984
7 HNO ₃ + Dust → HNO ₃ (d) + Dust	f	1×10 ⁻⁸			Schwartz and White 1981; Schwartz 1984
8 HNO ₃ (d) → HNO ₃	g	1×10 ¹⁵	8700	15.4	Schwartz and White 1981; Schwartz 1984
9 HONO + Dust → HONO(d) + Dust	f	1×10 ⁻⁸			Becker et al. 1996
10 HONO(d) → HONO	g	1×10 ¹⁰	4900	0	Becker et al. 1996
11 N ₂ O ₅ + Dust → HNO ₃ (d) + Dust	f	7.3×10 ⁻³			Wagner et al. 2009
Dust phase					
12 Dust + hν → Dust + e _h		j[ATD]			this study (Sect. 3.2.3)
13 e _h → energy	h	1×10 ⁻²			this study (Sect. 3.2.3)
14 e _h + O ₂ → OH(d)	i	1×10 ⁻²²	2.3RH		this study (Sect. 3.2.3)
15 SO ₂ (d) → SO ₄ ²⁻ (d)	h	5×10 ⁻⁶			this study (Sect. 3.2.2)
16 SO ₂ (d) + OH(d) → SO ₄ ²⁻ (d)	h	1×10 ⁻¹²			this study (Sect. 3.2.4)
17 SO ₂ (d) + O ₃ (d) → SO ₄ ²⁻ (d) + O ₂	h	2×10 ⁻¹¹			this study (Sect. 3.3.1)
18 e _h + O ₃ (d) → OH(d) + O ₂	h	1×10 ⁻¹²			this study (Sect. 3.3.1)
19 NO ₂ (d) → NO ₃ ⁻ (d)	h	6×10 ⁻⁵			this study (Sect. 3.3.2)
20 e _h + NO ₂ (d) → HONO(d)	h	6×10 ⁻¹²			this study (Sect. 3.3.2)
21 HONO(d) + hν → OH(d) + NO		j[HONO]			Stockwell and Calvert, 1978; Atkinson et al., 1997
22 NO ₂ (d) + OH(d) → NO ₃ ⁻ (d)	h	1×10 ⁻¹⁰			this study (Sect. 3.3.2)

Table S1. (continued)

Reaction	Rate constant ^a	k_1	k_2	k_3	Note
23 $\text{NO}_3^-(\text{d}) + \text{Salt}(\text{d}) \rightarrow \text{NO}_3^-(\text{d_salt})$	h	1×10^{-12}			this study (Sect. 3.3.2)
24 $\text{SO}_4^{2-}(\text{d}) + \text{Salt}(\text{d}) \rightarrow \text{SO}_4^{2-}(\text{d_salt})$	h	5×10^{-13}			this study (Sect. 3.3.2)
25 $\text{NO}_3^-(\text{d_salt}) + \text{SO}_4^{2-}(\text{d}) \rightarrow \text{SO}_4^{2-}(\text{d_salt})$	h	1×10^{-13}			this study (Sect. 3.3.2)
Reaction	Rate constant ^a	Note			
		Wall loss ^j			
1 $\text{SO}_2 \rightarrow$		$(1.3\text{RH} + 3.3) \times 10^{-6}$			For indoor chamber simulation; measured
2 $\text{O}_3 \rightarrow$		7×10^{-5}			For indoor chamber simulation; Chen and Jang, 2012
3 $\text{SO}_2 \rightarrow$		$(0.7\text{RH} + 1.7) \times 10^{-6}$			For outdoor chamber simulation; estimated
4 $\text{O}_3 \rightarrow$		3.5×10^{-5}			For outdoor chamber simulation; estimated
5 $\text{Dust} \rightarrow$		1×10^{-5}			Measured
6 $\text{SO}_4^{2-}(\text{aq}) \rightarrow$		5×10^{-6}			Measured

^aThe unit of reaction rate constants is s^{-1} for first-order reactions, $\text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}$ for second-order reactions and $\text{cm}^6 \text{molecule}^{-2} \text{s}^{-1}$ for third order reactions. The unit of the rate constants for the dust sorption reactions is $\text{m}^3 \text{m}^{-2} \text{s}^{-1}$.

^b The rate constant parameters of SO_2 oxidation in gas phase are taken from previous studies as shown in note of each reactions and can be also found in Chen and Jang (2012). T (K) is the temperature.

^c $V = N_A \times V(\text{aq})$, where $N_A (6.022 \times 10^{23} \text{ molecule mol}^{-1})$ is the Avogadro constant and $V(\text{aq}) (\text{L cm}^{-3})$ is the volume concentration of inorganic salt seeded aqueous phase in the air. The unit of the chemical species in the aqueous phase is mole per cm^3 of air for the model simulation. The rate constant parameters of reactions in aqueous phases are updated from previous studies (Liang et al., 1999). The detailed citation of each reactions was shown in the notes. The concentration of $V(\text{aq})$, $\text{H}_2\text{O}(\text{aq})$, H^+ and OH^- are calculated using E-AIM II (Clegg et al., 1998; Wexler and Clegg, 2002; Clegg and Wexler, 2011).

^d The partitioning rate constant of gas to the aqueous phase is derived from Henry constant (mol atm^{-1}). ρ_{in} is the density of the inorganic salt seeded aerosol and is calculated using E-AIM II (Clegg et al., 1998; Wexler and Clegg, 2002; Clegg and Wexler, 2011).

^e The unit of dust for the model is mass concentration ($\mu\text{g m}^{-3}$). During simulation, the concentration of dust is multiplied by a factor of 2.45×10^{10} to have same magnitude with other gaseous species.

^f Rate constant $k = k_1 \sqrt{8 R T / (\pi M W)} f_{dust,S,M} / 4$, where $f_{dust,S,M} = 3.066 \times 10^{-6} \text{ (m}^2 \mu\text{g}^{-1}\text{)}$, R = 8.314 is the ideal gas constant and MW is the molecule weight of chemical species.

^g Rate constant $k = k_1 \exp\left(-\frac{k_2}{T}\right) / (F_{\text{water}}(1 + k_3/[H^+]))$, where F_{water} is calculated using Eq. (8). $[H^+]$ is the concentration of proton and is dynamically calculated using E-AIM II. (Clegg et al., 1998; Wexler and Clegg, 2002; Clegg and Wexler, 2011).

5 h Rate constant $k = k_1$.

i Rate constant $k = k_1 \exp(k_2)$.

j The wall loss factors for the model simulation are only valid for the indoor and outdoor chambers used this study. The loss factors of gases and particles may be varied for different chamber systems.

Table S2. Calculation of the characteristic time of the major processes and reactions

Type of process	Characteristic time	Aqueous phase system	Dust system
r : the particle radius D_g : diffusion coefficient in gas D_l : diffusion coefficient in aqueous phase H : Henry's constant α : the mass accommodation coefficient (0.5) u_{av} is the mean thermal speed.		$r = 50 \text{ nm}$ $k_{SO2,g} = 1 \times 10^{-12} \text{ s}^{-1} \text{ molecule}^{-1} \text{ cc}$ $[\text{OH}] = 1 \times 10^6 \text{ molecules cc}^{-1}$ $k_{HSO3} = 3 \times 10^{-3} \text{ s}^{-1} \text{ molecule}^{-1} \text{ cc}$ $[\text{OH}]_{aq} = 0.1 \text{ molecules cc}^{-1}$	$r = 350 \text{ nm} \text{ (average)}$ $r_{dust,aq}$: the average thickness of the water layer on dust particles (40 nm) $k_{SO2,g} = 1 \times 10^{-12} \text{ s}^{-1} \text{ molecule}^{-1} \text{ cc}$ $[\text{OH}] = 1 \times 10^6 \text{ molecules cc}^{-1}$ $k_{SO2,dust} = 1 \times 10^{-12} \text{ s}^{-1} \text{ molecule}^{-1} \text{ cc}$ $[\text{OH}]_{aq} = 2 \times 10^9 \text{ molecules cc}^{-1}$
Gas diffusion	$\frac{r^2}{\pi^2 D_g}$	$2.4 \times 10^{-11} \text{ s}$	$2.1 \times 10^{-10} \text{ s}$
Diffusion in aqueous phase	$\frac{r_{aq}^2}{\pi^2 D_l}$	$1.9 \times 10^{-7} \text{ s}$	
Diffusion in the water layer on dust	$\frac{r_{dust,aq}^2}{\pi^2 D_l}$		$1.2 \times 10^{-7} \text{ s}$
Equilibrium between gas and particle	$D_l \left(\frac{4HRT}{\alpha u_{av}} \right)^2$	$7.1 \times 10^{-10} \text{ s}$	$7.1 \times 10^{-10} \text{ s}$
Reaction in gas phase	$\frac{1}{[\text{OH}] k_{SO2,g}}$	$1 \times 10^6 \text{ s}$	$1 \times 10^6 \text{ s}$
Reaction in aqueous phase	$\frac{1}{[\text{OH}]_{aq} k_{HSO3,aq}}$	$2 \times 10^3 \text{ s}$	
Reaction in dust phase	$\frac{1}{[\text{OH}]_{dust} k_{SO2,dust}}$		$5 \times 10^2 \text{ s}$

The characteristic time of the uptake process of tracers into aqueous phase or dust phase is calculated for gas-phase diffusion, liquid phase diffusion, establishing equilibrium at the interface and the reactions in gas, aqueous, and dust phases (Finlayson-Pitts and Pitts Jr, 1999).

For both the aqueous system and the dust system, the characteristic time of all reactions in gas and particles are much greater than diffusion in gas or particle phases and equilibrium processes (partitioning and dissociation of acids). Thus, the reactions of chemical species are not affected by the time reached to equilibrium or diffusion processes. In the model, both absorption and desorption rates of chemical species were set to much faster than their reaction rates in all three phase (last paragraph in Section 3.1.2). Furthermore, the time of diffusion in liquid phase is longer than both gas diffusion and the time for reaching to equilibrium as shown in Table S2.

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