Supplementary materials for

A Comprehensive Characterization of Empirical Parameterizations for OH Exposure in the Aerodyne Potential Aerosol Mass Oxidation Flow Reactor (PAM-OFR)

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Tables.

Table S1: List of OFR185 trace-gas decay experiments under different conditions. SO_2 or CO was used as the source of external OH reactivity (OHR_{ext}). Each set of experiments was performed under 5–9 lamp intensity settings.

Experiment ID	Species	Initial concentration(ppb)	OHR_{ext} (s^{-1})	Residence time (s)	Water vapor mixing ratio (%)
1		182.8	4.27	33.3	0.58
2		191.0	4.46	33.3	0.63
3		193.2	4.52	33.3	0.64
4		274.0	6.40	99.8	0.79
5		291.0	6.80	99.8	0.69
6		331.0	7.74	295.6	1.60
7		366.0	8.55	181.4	1.55
8		379.4	8.87	33.3	0.63
9		380.3	8.89	33.3	1.05
10	SO_2	383.1	8.96	33.3	0.87
11		489.4	11.44	61.4	0.62
12		513.0	11.99	199.5	0.66
13		650.0	15.19	181.4	2.72
14		750.0	17.53	181.4	1.98
15		789.1	18.45	33.3	0.74
16		973.2	22.75	33.3	1.19
17		8556.4	197.98	61.4	0.52
18		8556.4	200.00	33.3	0.38
19		8718.6	203.79	33.3	0.53
20		10247.8	60.58	33.3	1.15
21		12298.2	72.70	33.3	0.86
22	CO	103238.4	610.27	33.3	0.95
23		103852.8	613.91	33.3	0.86
24		207445.7	1226.27	33.3	0.97
25		207496.6	1226.58	33.3	0.89

Table S2: List of OFR254 trace-gas decay experiments under different conditions. SO_2 or CO was used as the source of OHR_{ext}. Each set of experiments was performed under 5–9 lamp intensity settings.

Experiment ID	Species	Initial concentration (ppb)	OHR_{ext} (s^{-1})	Input O_3 concentration (ppm)	Residence time (s)	Water vapor mixing ratio (%)
1		286.2	6.69	4.27	69.6	1.65
2		283.3	6.62	5.91	69.0	2.46
3		283.8	6.63	6.17	69.0	0.99
4		289.9	6.78	6.30	69.0	1.52
5		575.5	13.45	6.20	69.0	1.07
6		575.2	13.44	6.08	69.0	2.45
7		583.5	13.64	6.15	69.0	1.62
8		868.6	20.30	6.23	69.0	2.22
9		874.7	20.45	6.05	69.0	1.57
10		868.9	20.31	6.32	69.0	0.97
11		454.9	10.63	7.77	69.0	0.96
12		450.2	10.52	8.16	69.0	2.17
13		450.7	10.53	6.58	69.0	1.41
14		737.9	17.25	8.32	69.0	0.88
15	SO_2	746.8	17.46	7.77	69.0	2.20
16		747.0	17.46	9.38	69.0	1.50
17		204.0	4.77	2.62	34.4	2.11
18		201.9	4.72	3.00	34.4	1.32
19		196.9	4.60	2.90	34.4	0.94
20		282.6	6.61	6.07	34.4	0.79
21		572.9	13.39	6.11	34.4	0.82
22		908.6	21.24	6.08	34.4	0.78
23		204.7	4.78	4.47	43.7	0.86
24		402.8	9.41	5.47	47.4	2.14
25		459.9	10.75	5.34	54.0	1.91
26		840.2	19.64	9.82	111.5	1.74
27		262.7	6.14	8.23	70.9	2.27
28		430.8	10.07	8.19	70.6	2.23
29		260.1	6.08	13.17	69.6	2.38
30		511.4	11.95	19.39	125.5	2.61

| Experiment ID	Species	Initial concentration (ppb)	OHR$_{ext}$ (s^{-1})	Input O$_3$ concentration (ppm)	Residence time (s)	Water vapor mixing ratio (%)
31		4909.4	29.02	3.15	19.8	0.91
32		4685.6	27.70	5.06	37.4	0.83
33		4958.3	29.31	4.13	47.1	0.78
34	CO	4829.8	28.55	5.59	69.4	2.20
35		4358.0	25.76	2.95	34.5	1.78
36		5034.5	29.76	4.82	46.8	2.18
37		4438.5	26.24	12.95	95.2	2.25

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Table S3: In OFR185 mode, the parameters a–f for the $OH_{exp, est}$ estimation were obtained from different data sets.

| OFR185	Figure #	Data sets	FP	Coefficient					
				a	b	c	d	e	f
Residence time	Fig. 1a1	short t	$FP_{st, 185}$	4.2566	0.57973	-0.062233	0.47836	0.0027988	0.55255
	Fig. 1a2	adding long t							
	Fig. 1a3		$FP_{et, 185}$	4.5772	0.58603	-0.10617	0.40819	0.004321	0.50352
Water vapor mixing ratio	Fig. 1b1	low H_2O	$FP_{lH2O, 185}$	5.5822	0.62134	-0.23848	0.27915	0.0071196	0.42689
	Fig. 1b2	adding high H_2O							
	Fig. 1b3		$FP_{eH2O, 185}$	4.2899	0.70966	-0.21378	0.23242	0.0052289	0.39371
Output O_3 concentration	Fig. 1c1	low $O_{3, out}$	$FP_{lO3, 185}$	3.3154	2.3046	-1.74	0.033076	0.0061601	0.29402
	Fig. 1c2	adding high $O_{3, out}$							
	Fig. 1c3		$FP_{eO3, 185}$	3.5229	2.2995	-1.7422	0.027553	0.0050063	0.29182
External OHR	Fig. 2a	low OHR_{ext}	$FP_{lOHR, 185}$	3.2404	0.74398	-0.13922	0.26786	0.0026332	0.4917
	Fig. 2b	adding high OHR_{ext}							
	Fig. 2c		$FP_{eOHR, 185}$	3.5103	0.62481	-0.079114	0.36805	0.0041654	0.38722
OHR source	Fig. 3a	SO_2	$FP_{SO2, 185}$	3.2759	0.65745	-0.10638	0.23087	0.0050212	0.24198
	Fig. 3b	CO	$FP_{CO, 185}$	4.1575	0.55935	-0.86966	-0.17843	0.089848	-0.2993
	Fig. 3c	SO_2 + CO	$FP_{SO2\&CO, 185}$	2.1665	0.78424	-0.13214	0.089098	0.0036945	0.03358

Table S4: In OFR254 mode, the parameters a–c of the $OH_{exp, est}$ estimation were obtained from different data sets.

| OFR254	Figure #	Data sets	FP	Coefficient		
				a	b	c
External OHR	Fig. 4a1	low OHR_{ext}	$FP_{lOHR, 254}$	12.798	0.34588	0.085063
	Fig. 4a2	adding high OHR_{ext}				
	Fig. 4a3		$FP_{eOHR, 254}$	13.151	-17.172	0.12986
Input O_3 concentration	Fig. 4b1	low $O_{3, in}$	$FP_{lO3, 254}$	13.459	-19.285	0.11153
	Fig. 4b2	adding high $O_{3, in}$				
	Fig. 4b3		$FP_{eO3, 254}$	13.325	-19.393	0.12029
r_{O3}	Fig. 4c1	medium r_{O3}	$FP_{mrO3, 254}$	12.989	-9.9122	0.13684
	Fig. 4c2	adding extended r_{O3}				
	Fig. 4c3		$FP_{erO3, 254}$	13.213	-18.921	0.13111
OHR source	Fig. 5a	SO_2	$FP_{SO2, 254}$	13.145	-18.669	0.13316
	Fig. 5b	CO	$FP_{CO, 254}$	16.161	-92.945	0.11466
	Fig. 5c	$SO_2 + CO$	$FP_{SO2\&CO, 254}$	13.075	-15.698	0.13741

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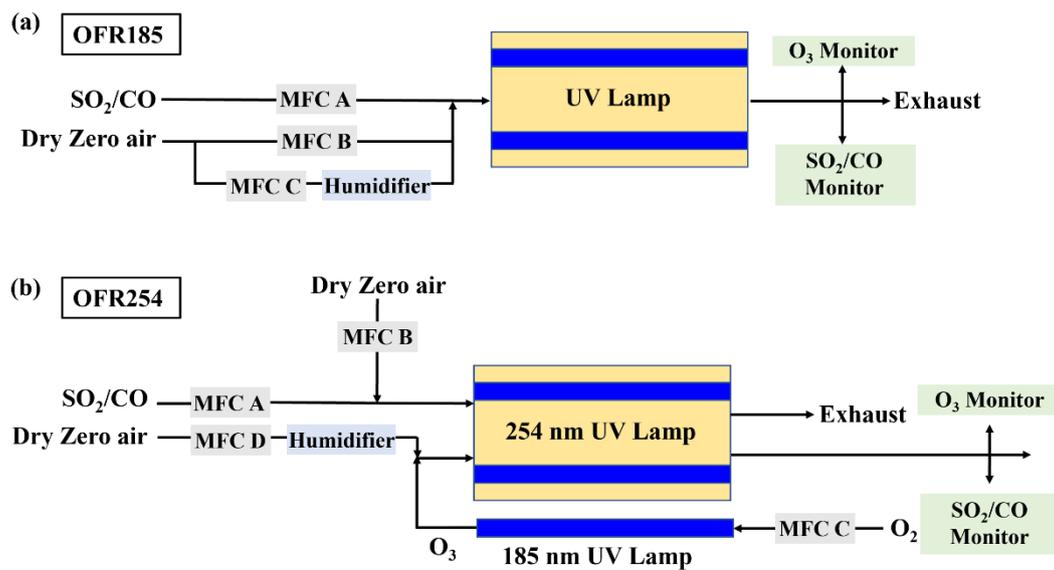
Figures.

Figure S1: The schematics of the PAM-OFR experimental setup for trace-gas decay experiments in (a) OFR185 mode and (b) OFR254 mode.
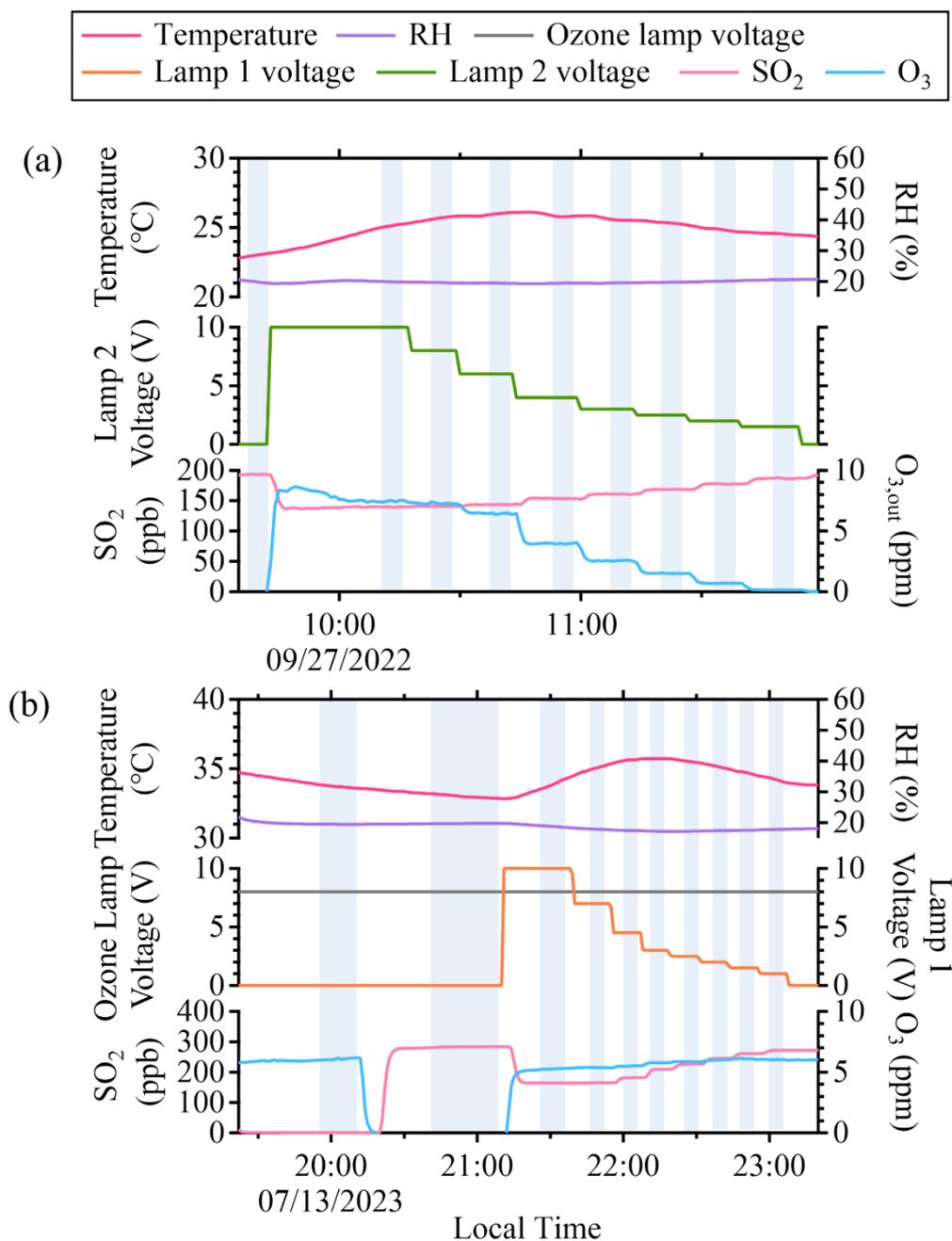
Figure S2: The examples of a set of experiments conducted in (a) the OFR185 mode and (b) the OFR254 mode, respectively. A set of experiments was operated with light voltage settings stepping decreasing from 10V to 0V. The highlighted areas indicate the periods when all conditions had reached a steady state and the tracer gas was sampled.

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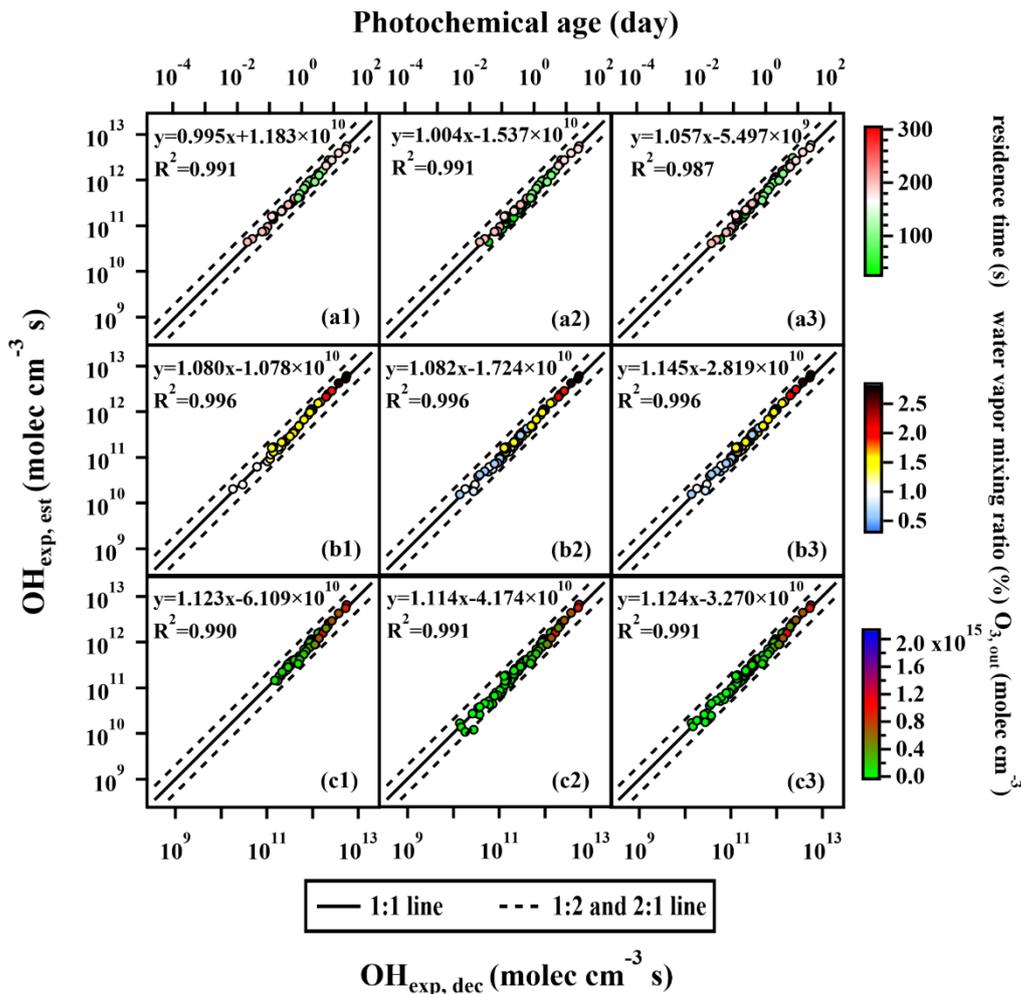
Figure S3: The regression results of $OH_{exp, est}$ and $OH_{exp, dec}$ when variations occurred in (a1–a3) residence time, (b1–b3) water vapor mixing ratio, and (c1–c3) output O_3 concentration under atmospheric relevant OHR_{ext} level (4–23 s^{-1}). Compared to panels a1, b1, and c1, panels a2, b2, and c2 respectively incorporated additional data points with lower t, H_2O, and $O_{3, out}$ values, but still utilized the fitting parameters *a–f* obtained from the higher condition range to estimate $OH_{exp, est}$. In panels a3, b3, and c3, all data points within the extended condition range were used to re-fit the parameters *a–f*, which were employed to estimate $OH_{exp, est}$.
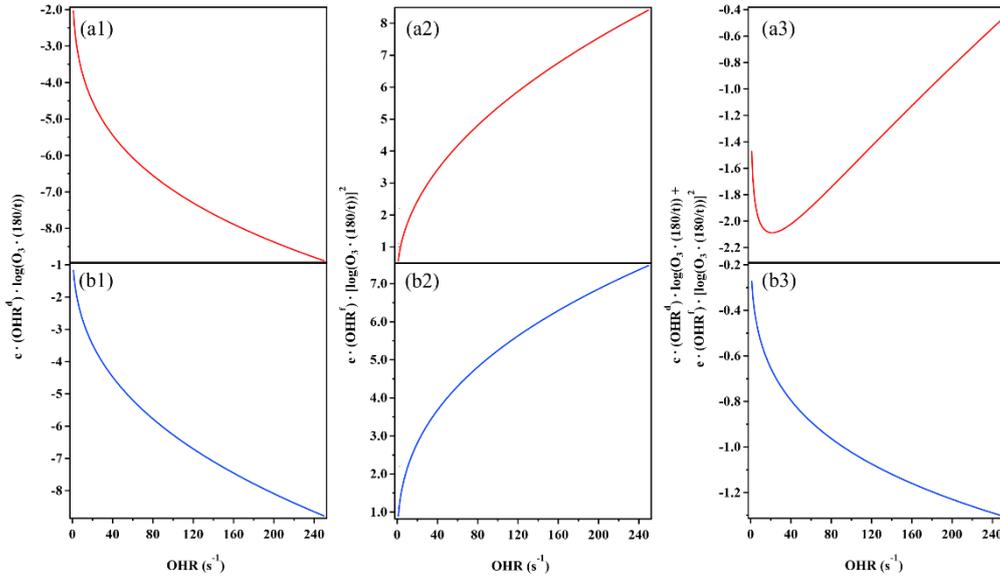
Figure S4: (a1–a3) The variations of $c \times \mathrm{OHR}_{ext}^{d} \times \log(O_{3,\,out} \times 180/t)$, $e \times \mathrm{OHR}_{ext}^{f} \times [\log(O_{3,\,out} \times 180/t)]^2$ and their sum with respect to OHR_{ext} when using the fitted values of c–f (-0.13922, 0.26786, 0.0026332, 0.4917) obtained from the low OHR_{ext} data points. (b1–b3) The variations of $c \times \mathrm{OHR}_{ext}^{d} \times \log(O_{3,\,out} \times 180/t)$, $e \times \mathrm{OHR}_{ext}^{f} \times [\log(O_{3,\,out} \times 180/t)]^2$ and their sum with respect to OHR_{ext} when using the fitted values of c–f (-0.079114, 0.36805, 0.0041654, 0.38722) obtained from the data points with a wider range of OHR_{ext} condition.