Supplement to Technical Note: Effect of varying λ = 185 and 254 nm photon flux ratios on radical generation in oxidation flow reactors

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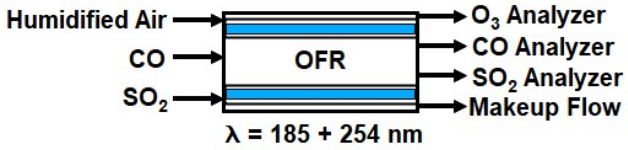

Figure S1. Simplified schematic of experimental setup used in this study.

Figure S2. Photo to of lamp type B used in this study. Heat shrink tubing applied to the external surface of the Hg lamp quartz caused equivalent reduction in I_{185} and I_{254}.

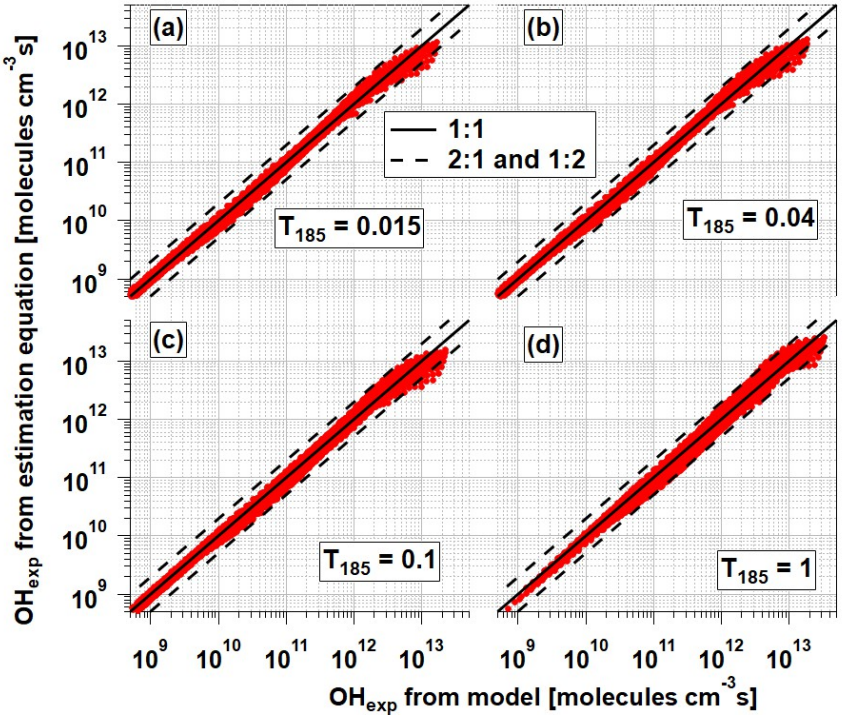

Figure S3. OH_{exp} calculated from the estimation equation (Eq. 1) as a function of OH_{exp} calculated from the full OFR185 KinSim mechanism (Table S1) for lamp types (a) E, (b) D and G, (c) C and F, and (d) A and B. Solid and dashed lines correspond to the 1:1 and the 1:2 and 2:1 lines, respectively. Estimation equation fit coefficients are shown in Table 1.

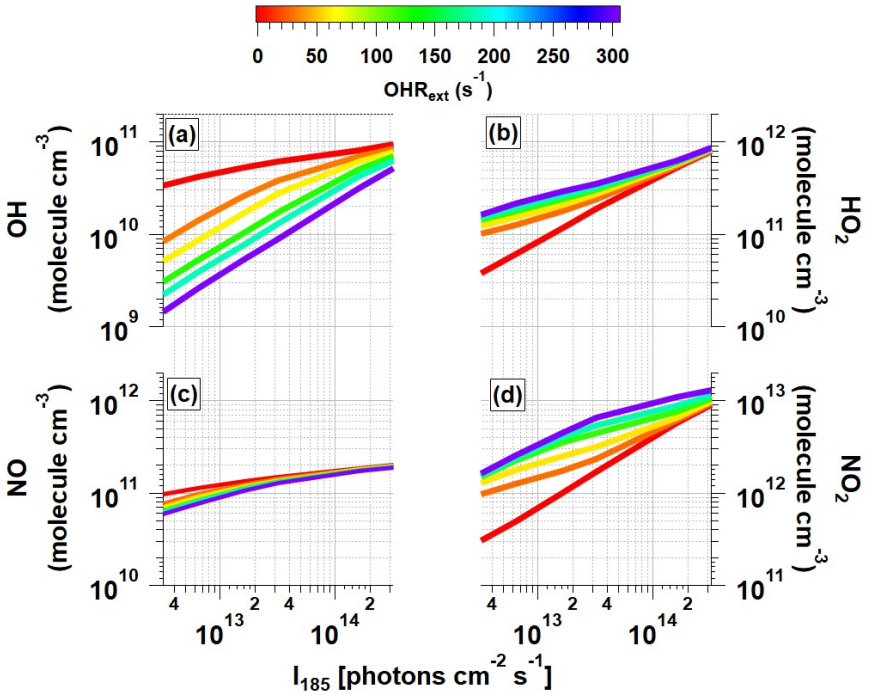

Figure S4. Concentrations of (a) OH, (b) HO_2, (c) NO, and (d) NO_2 as a function of I_{185} and OHR_{ext} calculated using the OFR185 KinSim mechanism at the following base case OFR185 conditions: $[H_2O] = [N_2O] = 2\%$, $I_{254} = 3.2\times10^{15}$ photons cm^{-2} s^{-1}, and τ_{OFR} = 124 s.

Table S1: KinSim mechanism used to model OFR185 radical chemistry (Peng and Jimenez, 2020).

Reactant 1	Reactant 2	Product 1	Product 2	Product 3	A_∞	E_∞	n_∞	A_0	E_0	n_0	F_c	f_0	g
$O(^1D)$	H_2O	OH	OH		1.63E-10	-60	0	0	0	0	0	1	0
$O(^1D)$	N_2	$O(^3P)$	N_2		2.15E-11	-110	0	0	0	0	0	1	0
$O(^1D)$	CO_2	$O(^3P)$	CO_2		7.5E-11	-115	0	0	0	0	0	1	0
$O(^1D)$	O_2	$O(^3P)$	O_2		3.3E-11	-55	0	0	0	0	0	1	0
$O(^1D)$	O_3	O_2	O_2		1.2E-10	0	0	0	0	0	0	1	0
$O(^1D)$	O_3	O_2	$O(^3P)$	$O(^3P)$	1.2E-10	0	0	0	0	0	0	1	0
$O(^1D)$	H_2	OH	H		1.2E-10	0	0	0	0	0	0	1	0
$O(^3P)$	OH	O_2	H		1.8E-11	-120	0	0	0	0	0	1	0
$O(^3P)$	HO_2	OH	O_2		3E-11	-200	0	0	0	0	0	1	0
$O(^3P)$	H_2O_2	OH	HO_2		1.4E-12	2000	0	0	0	0	0	1	0
$O(^3P)$	O_3	O_2	O_2		8E-12	2060	0	0	0	0	0	1	0
H	O_3	OH	O_2		1.4E-10	470	0	0	0	0	0	1	0
OH	O_3	HO_2	O_2		1.7E-12	940	0	0	0	0	0	1	0
HO_2	NO	OH	NO_2		3.3E-12	-270	0	0	0	0	0	1	0
HO_2	O_3	OH	O_2	O_2	1E-14	490	0	0	0	0	0	1	0
OH	HO_2	H_2O	O_2		4.8E-11	-250	0	0	0	0	0	1	0
H	HO_2	OH	OH		7.2E-11	0	0	0	0	0	0	1	0
H	HO_2	$O(^3P)$	H_2O		1.6E-12	0	0	0	0	0	0	1	0
H	HO_2	O_2	H_2		6.9E-12	0	0	0	0	0	0	1	0
OH	H_2	H_2O	H		2.8E-12	1800	0	0	0	0	0	1	0
OH	OH	H_2O	$O(^3P)$		1.8E-12	0	0	0	0	0	0	1	0
NO	O_3	NO_2	O_2		3E-12	1500	0	0	0	0	0	1	0
NO_2	O_3	NO_3	O_2		1.2E-13	2450	0	0	0	0	0	1	0
OH	H_2O_2	H_2O	HO_2		1.8E-12	0	0	0	0	0	0	1	0
HO_2	NO_2	HNO_4			2.9E-12	0	1.1	2E-31	0	3.4	0	1	0
OH	HNO_4	H_2O	O_2	NO_2	1.3E-12	-380	0	0	0	0	0	1	0
$O(^1D)$	N_2	N_2O			0	0	0	2.8E-36	0	0.9	0	1	0
OH	NO_2	HNO_3			2.9E-11	0	1.1	1.8E-30	0	3	0	1	0
$O(^3P)$	O_2	O_3			0	0	0	6E-34	0	2.4	0	1	0
H	O_2	HO_2			7.5E-11	0	-0.2	4.4E-32	0	1.3	0	1	0
OH	OH	H_2O_2			2.6E-11	0	0	6.9E-31	0	1	0	1	0

OH	SO_2	HSO_3			1.6E-12	0	0	3.3E-31	0	4.3	0	1	0
HSO_3	O_2	HO_2	SO_3		1.3E-12	300	0	0	0	0	0	1	0
OH	HNO_3	H_2O	NO_3		2.4E-14	-460	0	6.5E-34	-1335	0	0	1	0
O_2	HV185	$O(^3P)$	$O(^3P)$		1.1E-20	0	0	0	0	0	0	1	0
O_3	HV254	O_2	$O(^1D)$		1.03E-17	0	0	0	0	0	0	1	0
H_2O_2	HV185	HO_2			1E-19	0	0	0	0	0	0	1	0
H_2O_2	HV254	OH			6.7E-20	0	0	0	0	0	0	1	0
HO_2	HV254	OH			2.63E-19	0	0	0	0	0	0	1	0
HO_2	HV185	OH			3.68E-18	0	0	0	0	0	0	1	0
H_2O	HV185	OH	H		6.78E-20	0	0	0	0	0	0	1	0
HO_2	HO_2	H_2O_2	O_2		3E-13	-600	0	2.1E-33	-1000	0	0	1	0
$O(^3P)$	NO	NO_2			3E-11	0	0	9E-32	0	1.5	0	1	0
$O(^3P)$	NO_2	NO	O_2		5.1E-12	-210	0	0	0	0	0	1	0
$O(^3P)$	NO_2	NO_3			2.2E-11	0	0.7	2.5E-31	0	1.8	0	1	0
$O(^3P)$	NO_3	O_2	NO_2		1E-11	0	0	0	0	0	0	1	0
OH	NO	HNO_2			3.6E-11	0	0.1	7E-31	0	2.6	0	1	0
OH	HNO_2	H_2O	NO_2		1.8E-11	390	0	0	0	0	0	1	0
HO_2	NO_3	OH	NO_2	O_2	3.5E-12	0	0	0	0	0	0	1	0
HO_2	NO_3	NO	NO_2	O_2	4.5E-14	1260	0	0	0	0	0	1	0
NO_2	NO_3	N_2O_5			1.4E-12	0	0.7	2E-30	0	4.4	0	1	0
NO_3	NO_3	NO_2	NO_2	O_2	8.5E-13	2450	0	0	0	0	0	1	0
O_3	HNO_2	O_2	HNO_3		2.5E-19	0	0	0	0	0	0	1	0
N_2O_5	H_2O	HNO_3	HNO_3		1E-21	0	0	0	0	0	0	1	0
NO_2	HV185	NO	$O(^1D)$		6.882E-18	0	0	0	0	0	0	1	0
NO_2	HV185	NO	$O(^3P)$		1.05E-20	0	0	0	0	0	0	1	0
N_2O	HV185	N_2	$O(^1D)$		1.43E-19	0	0	0	0	0	0	1	0
HNO_4		NO_2	HO_2		6E+15	11170	0	4.1E-05	10650	0	0.4	1	0
N_2O_5		NO_2	NO_3		9.7E+14	11000	0.1	0.0013	11000	3.5	0.35	1	0
N_2O	$O(^1D)$	N_2	O_2		4.64E-11	-20	0	0	0	0	0	1	0
N_2O	$O(^1D)$	NO	NO		7.26E-11	-20	0	0	0	0	0	1	0
OH	CO	HO_2	CO_2		1.5E-13	0	-0.6	0	0	0	0	1	0
OH	CO	HOCO			1.1E-12	0	-1.3	5.9E-33	0	0.4	0	1	0

References

Peng, Z. and Jimenez, J. L.: Radical chemistry in oxidation flow reactors for atmospheric chemistry research, Chem. Soc. Rev., http://dx.doi.org/10.1039/C9CS00766K, 2020.