

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

Jake Rowe^{1,+,*}, Andrew Lambe^{2,*}, and William Brune¹

¹Department of Meteorology and Atmospheric Science, Pennsylvania State University, University Park, PA, USA

²Center for Aerosol and Cloud Chemistry, Aerodyne Research Inc., Billerica, MA, USA

⁺Now at: Department of Chemistry, University of Colorado, Boulder, CO, USA

^{*}These authors contributed equally to this work.

Correspondence: Andrew T. Lambe (lambe@aerodyne.com)

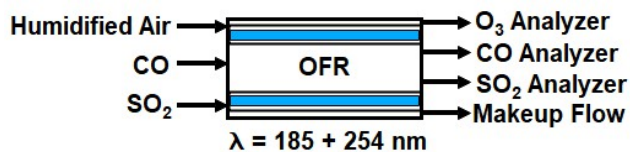


Figure S1. Simplified schematic of experimental setup used in this study.



Figure S2. Photo 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} .

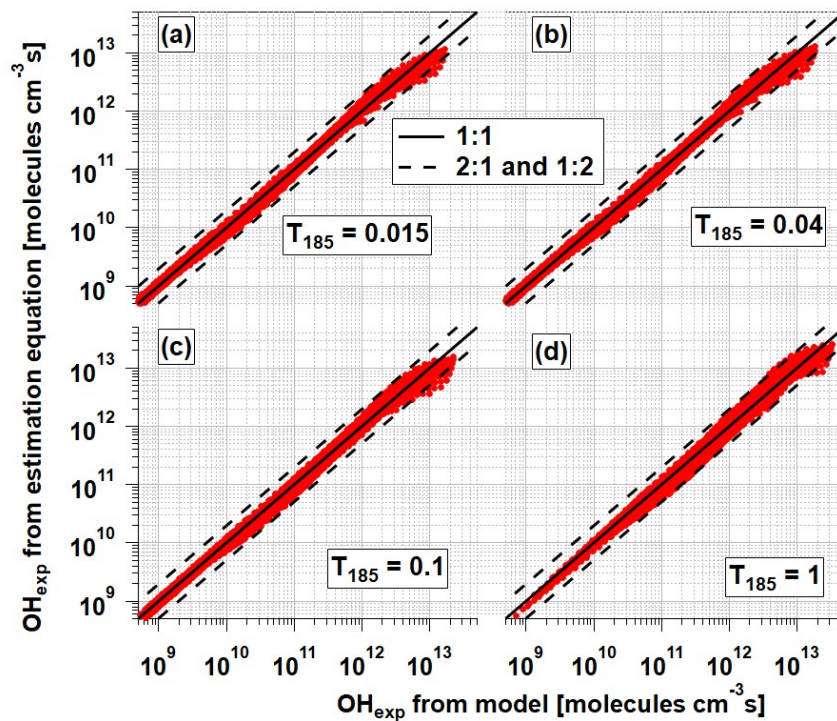


Figure S3. OH_{exp} calculated from the estimation equation (Eq. 1) as a function of OH_{exp} calculated from the full OFR185 KinSim mechanism (Table S1) for lamp types (a) E, (b) D and G, (c) C and F, and (d) A and B. Solid and dashed lines correspond to the 1:1 and the 1:2 and 2:1 lines, respectively.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

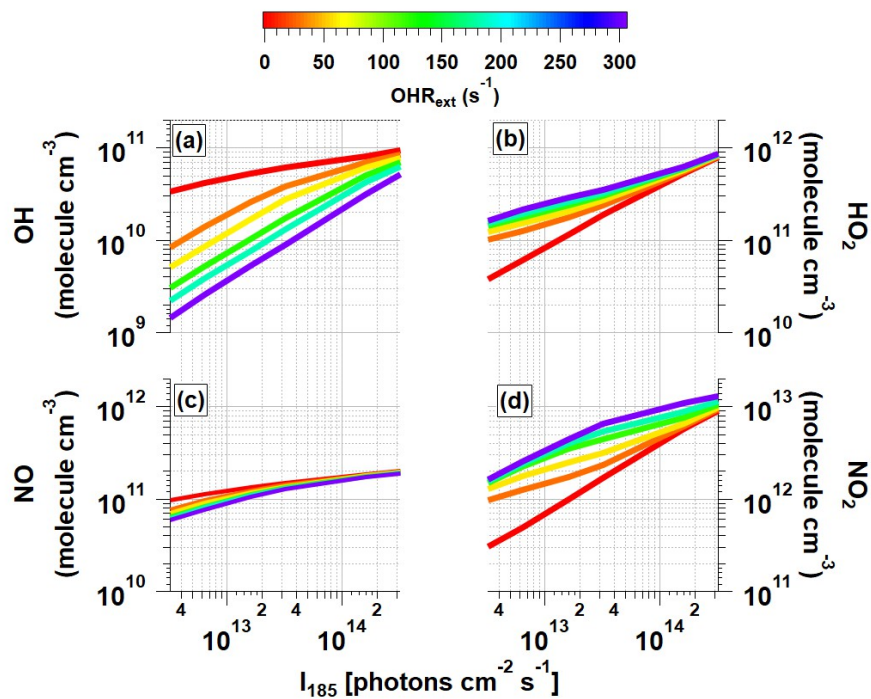


Figure S4. Concentrations of (a) OH, (b) HO₂, (c) NO, and (d) NO₂ as a function of I_{185} and OHR_{ext} calculated using the OFR185 KinSim mechanism at the following base case OFR185 conditions: $[\text{H}_2\text{O}] = [\text{N}_2\text{O}] = 2\%$, $I_{254} = 3.2 \times 10^{15} \text{ photons cm}^{-2} \text{ s}^{-1}$, and $\tau_{\text{OFR}} = 124 \text{ s}$.

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(¹ D)	H ₂ O	OH	OH		1.63E-10	-60	0	0	0	0	0	1	0
O(¹ D)	N ₂	O(³ P)	N ₂		2.15E-11	-110	0	0	0	0	0	1	0
O(¹ D)	CO ₂	O(³ P)	CO ₂		7.5E-11	-115	0	0	0	0	0	1	0
O(¹ D)	O ₂	O(³ P)	O ₂		3.3E-11	-55	0	0	0	0	0	1	0
O(¹ D)	O ₃	O ₂	O ₂		1.2E-10	0	0	0	0	0	0	1	0
O(¹ D)	O ₃	O ₂	O(³ P)	O(³ P)	1.2E-10	0	0	0	0	0	0	1	0
O(¹ D)	H ₂	OH	H		1.2E-10	0	0	0	0	0	0	1	0
O(³ P)	OH	O ₂	H		1.8E-11	-120	0	0	0	0	0	1	0
O(³ P)	HO ₂	OH	O ₂		3E-11	-200	0	0	0	0	0	1	0
O(³ P)	H ₂ O ₂	OH	HO ₂		1.4E-12	2000	0	0	0	0	0	1	0
O(³ P)	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 ₂ O	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(³ P)	H ₂ O		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 ₂ O	H		2.8E-12	1800	0	0	0	0	0	1	0
OH	OH	H ₂ O	O(³ P)		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 ₂ O ₂	H ₂ O	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 ₂ O	O ₂	NO ₂	1.3E-12	-380	0	0	0	0	0	1	0
O(¹ D)	N ₂	N ₂ O			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(³ P)	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 ₂ O 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 ₂ O	NO ₃		2.4E-14	-460	0	6.5E-34	-1335	0	0	1	0
O ₂	HV185	O(³ P)	O(³ P)		1.1E-20	0	0	0	0	0	0	1	0
O ₃	HV254	O ₂	O(¹ D)		1.03E-17	0	0	0	0	0	0	1	0
H ₂ O ₂	HV185	HO ₂			1E-19	0	0	0	0	0	0	1	0
H ₂ O 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 ₂ O	HV185	OH	H		6.78E-20	0	0	0	0	0	0	1	0
HO ₂	HO ₂	H ₂ O ₂	O ₂		3E-13	-600	0	2.1E-33	-1000	0	0	1	0
O(³ P)	NO	NO ₂			3E-11	0	0	9E-32	0	1.5	0	1	0
O(³ P)	NO ₂	NO	O ₂		5.1E-12	-210	0	0	0	0	0	1	0
O(³ P)	NO ₂	NO ₃			2.2E-11	0	0.7	2.5E-31	0	1.8	0	1	0
O(³ P)	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 ₂ O	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 ₂ O 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 ₂ O ₅	H ₂ O	HNO ₃	HNO ₃		1E-21	0	0	0	0	0	0	1	0
NO ₂	HV185	NO	O(¹ D)		6.882E-18	0	0	0	0	0	0	1	0
NO ₂	HV185	NO	O(³ P)		1.05E-20	0	0	0	0	0	0	1	0
N ₂ O	HV185	N ₂	O(¹ D)		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 ₂ O ₅		NO ₂	NO ₃		9.7E+14	11000	0.1	0.0013	11000	3.5	0.35	1	0
N ₂ O	O(¹ D)	N ₂	O ₂		4.64E-11	-20	0	0	0	0	0	1	0
N ₂ O	O(¹ D)	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.