Supplementary Information for:

Volatile organic compound conversion by ozone, hydroxyl radicals, and nitrate radicals in residential indoor air: Magnitudes and impacts of oxidant sources

Michael S. Waring and J. Raymond Wells

Table S1. Median residential volatile organic compound (VOC) concentrations from Logue et al. (2011); rate constant data from Atkinson and Arey (2003) and Master Chemical Mechanism v3.2 (Bloss et al., 2005; Jenkin et al., 1997, 2003; Saunders et al., 2003); and molar yields for hydroxyl radicals from Weschler and Shields (1996).

VOC j	Conc. j (ppb)	$k_{j\text{-O3}}$ (ppb^{-1} h^{-1})	$k_{j\text{-OH}}$ (ppb^{-1} h^{-1})	$k_{j\text{-NO3}}$ (ppb^{-1} h^{-1})	$Y_{OH,j}$ (-)	$k_{j\text{-O3}}C_j$ (h^{-1})	$k_{j\text{-OH}}C_j$ (h^{-1})	$k_{j\text{-NO3}}C_j$ (h^{-1})
1,1,1-trichloroethane	0.055	0	3.8E+02	0	0	0	2.1E+01	0
1,1,2,2-tetrachloroethane	0.0015	0	4.5E+01	0	0	0	6.6E-02	0
1,1-dichloroethene	0.00013	0	9.7E+02	0	0	0	1.2E-01	0
1,2,3-trimethylbenzene	0.081	0	2.9E+03	1.7E-01	0	0	2.4E+02	1.4E-02
1,2,3-trichlorobenzene	0.054	0	0	0	0	0	0	0
1,2,4-trimethylbenzene	0.57	8.9E-07	2.9E+03	1.6E-01	0	5.1E-07	1.6E+03	9.1E-02
1,2-dibromoethane	0.0013	0	2.0E+01	0	0	0	2.6E-02	0
1,2-dichlorobenzene	0.0017	0	3.7E+01	0	0	0	6.2E-02	0
1,2-dichloroethane	0.025	0	2.1E+01	0	0	0	5.3E-01	0
1,2-dichloropropane	0.0043	0	3.9E+01	0	0	0	1.7E-01	0
1,3,5-trimethylbenzene	0.12	0	5.0E+03	7.8E-02	0	0	6.1E+02	9.5E-03
1,3-butadiene	0.072	5.6E-04	5.9E+03	9.0E+00	0.08	4.0E-05	4.3E+02	6.5E-01
1,3-dichlorobenzene	0.025	0	6.4E+01	0	0	0	1.6E+00	0
1,4-dichlorobenzene	0.47	0	2.8E+01	0	0	0	1.3E+01	0
2,3-dimethylpentane	0.17	0	0	0	0	0	0	0
2,4-dimethylpentane	0.15	0	4.2E+02	1.3E-02	0	0	6.2E+01	1.9E-03
2-butoxyethanol	0.30	0	2.0E+03	4.1E-01	0	0	6.1E+02	1.2E-01
2-carene	0.0054	2.0E-02	7.1E+03	1.7E+03	0.85	1.1E-04	3.8E+01	9.1E+00
2-ethoxyethanol	0.017	0	1.6E+03	2.5E-01	0	0	2.8E+01	4.3E-03
2-ethyltoluene	0.10	0	1.1E+03	6.3E-02	0	0	1.1E+02	6.4E-03
2-methoxyethanol	0.039	0	1.1E+03	1.4E-01	0	0	4.2E+01	5.2E-03
2-methylhexane	0.44	0	6.1E+02	0	0	0	2.7E+02	0
2-methylpentane	0.45	0	4.7E+02	1.6E-02	0	0	2.1E+02	7.2E-03
2-propanol	1.3	0	4.5E+02	1.2E-01	0	0	6.1E+02	1.7E-01
3-carene	0.66	3.3E-03	7.8E+03	8.1E+02	0.85	2.2E-03	5.2E+03	5.4E+02
3-ethyltoluene	0.13	0	1.6E+03	4.0E-02	0	0	2.2E+02	5.4E-03
4-ethyltoluene	0.20	0	1.0E+03	7.6E-02	0	0	2.1E+02	1.5E-02
acetaldehyde	7.2	0	1.3E+03	2.4E-01	0	0	9.6E+03	1.7E+00
acetic acid	3.8	0	7.1E+01	0	0	0	2.7E+02	0
acetone	8.8	0	1.5E+01	2.7E-03	0	0	1.4E+02	2.4E-02
acrolein	0.37	2.6E-05	1.8E+03	2.8E-01	0	9.4E-06	6.5E+02	1.0E-01
acrylonitrile	0.028	0	3.6E+02	0	0	0	1.0E+01	0
a-pinene	2.2	7.7E-03	4.6E+03	5.5E+02	0.85	1.7E-02	1.0E+04	1.2E+03
benzaldehyde	0.67	0	1.1E+03	2.1E-01	0	0	7.3E+02	1.4E-01
benzene	0.66	8.9E-07	1.1E+02	2.7E-03	0	5.8E-07	7.1E+01	1.7E-03
b-pinene	0.22	1.3E-03	6.8E+03	2.2E+02	0.35	2.9E-04	1.5E+03	4.8E+01
bromodichloromethane	0.030	0	0	0	0	0	0	0
butanal	0.41	0	2.1E+03	9.8E-01	0	0	8.6E+02	4.0E-01
2-butanol	18	0	7.7E+02	1.9E-01	0	0	1.4E+04	3.4E+00
butylbenzene	0.015	0	0	0	0	0	0	0
carbon disulfide	0.042	0	2.6E+02	0	0	0	1.1E+01	0

carbon tetrachloride	0.091	0	1.1E-02	0	0	0	9.6E-04	0
chlorobenzene	0.030	0	6.8E+01	0	0	0	2.1E+00	0
chloroform	0.19	0	9.2E+00	0	0	0	1.7E+00	0
chloromethane	0.24	0	3.8E+00	0	0	0	9.3E-01	0
crotonaldehyde	0.16	1.4E-04	3.0E+03	5.3E-01	0.2	2.2E-05	4.7E+02	8.4E-02
cycloheptane	0.12	0	1.1E+03	0	0	0	1.4E+02	0
cyclohexane	0.46	0	6.2E+02	1.2E-02	0	0	2.9E+02	5.8E-03
decanal	0.14	0	0	2.0E+00	0	0	0	2.8E-01
decane	0.65	0	1.0E+03	2.5E-02	0	0	6.5E+02	1.6E-02
dibromochloromethane	0.0094	0	0	0	0	0	0	0
dichlorofluoromethane	0.78	0	2.7E+00	0	0	0	2.1E+00	0
d-limonene	2.5	1.8E-02	1.5E+04	1.1E+03	0.86	4.5E-02	3.7E+04	2.7E+03
dodecane	0.36	0	1.2E+03	0	0	0	4.3E+02	0
ethanol	85	0	2.8E+02	1.8E-01	0	0	2.4E+04	1.5E+01
ethylacetate	0.28	0	1.5E+02	0	0	0	4.1E+01	0
ethylbenzene	0.35	0	6.2E+02	1.1E-02	0	0	2.1E+02	3.7E-03
ethylcyclohexane	0.33	0	0	0	0	0	0	0
formaldehyde	19	0	7.9E+02	4.9E-02	0	0	1.5E+04	9.2E-01
freon 11	0.52	0	0	0	0	0	0	0
freon 113	0.065	0	0	0	0	0	0	0
glyoxal	1.1	0	9.2E+02	2.4E-01	0	0	1.0E+03	2.6E-01
heptane	0.61	0	6.1E+02	1.3E-02	0	0	3.8E+02	8.2E-03
hexanal	2.1	0	2.6E+03	8.3E-01	0	0	5.3E+03	1.7E+00
hexane	0.85	0	4.7E+02	9.8E-03	0	0	4.0E+02	8.3E-03
isobutane	9.7	0	1.9E+02	0	0	0	1.9E+03	0
isooctane	0.13	0	3.3E+02	0	0	0	4.2E+01	0
isoprene	0.72	1.1E-03	8.9E+03	6.2E+01	0.27	8.1E-04	6.4E+03	4.4E+01
isopropylbenzene	0.016	0	5.6E+02	1.2E-02	0	0	9.1E+00	2.0E-04
isovaleraldehyde	0.28	0	2.6E+03	2.4E-01	0	0	7.2E+02	6.7E-02
methyl ethyl ketone	1.2	0	9.8E+01	0	0	0	1.1E+02	0
methyl methacrylate	0.0012	0	2.3E+03	0	0	0	2.8E+00	0
methylcyclohexane	0.42	0	8.5E+02	0	0	0	3.6E+02	0
methylcylopentane	0.23	0	0	0	0	0	0	0
methylene chloride	0.32	0	1.3E+01	0	0	0	4.2E+00	0
methylglyoxal	0.92	0	1.2E+03	2.4E-01	0	0	1.1E+03	2.2E-01
methyl isobutyl ketone	0.073	0	1.3E+03	0.0E+00	0	0	9.2E+01	0.0E+00
methyl tert-butyl ether	1.7	0	2.6E+02	5.7E-02	0	0	4.3E+02	9.4E-02
nonane	0.27	0	8.7E+02	2.0E-02	0	0	2.3E+02	5.4E-03
octane	0.21	0	7.5E+02	1.7E-02	0	0	1.6E+02	3.6E-03
pentanal	0.51	0	2.5E+03	7.9E-01	0	0	1.3E+03	4.0E-01
propanal	0.76	0	1.7E+03	5.7E-01	0	0	1.3E+03	4.3E-01
propylbenzene	0.10	0	5.1E+02	1.2E-02	0	0	5.2E+01	1.3E-03
styrene	0.16	1.5E-03	5.1E+03	1.3E+02	0.37	2.5E-04	8.5E+02	2.2E+01
tetrachlorothene	0.21	0	0	0	0	0	0	0
toluene	4.8	0	5.1E+02	6.2E-03	0	0	2.5E+03	3.0E-02
trichloroethene	0.093	0	1.8E+02	0	0	0	1.6E+01	0
tridecane	0.23	0	1.3E+03	0	0	0	3.0E+02	0
undecane	0.63	0	1.1E+03	0	0	0	7.0E+02	0
xylene, o	0.30	0	1.2E+03	3.6E-02	0	0	3.6E+02	1.1E-02
xylene, m/p	0.99	8.9E-07	1.6E+03	3.2E-02	0	8.8E-07	1.6E+03	3.1E-02
					Sum =	**6.6E-02**	**1.5E+05**	**4.5E+03**

Table S2. Actual regression coefficients of natural log-transformed inputs regressed against the natural log-transformed outcome variables. See main text for variable and set definitions.

Outcome [a]	Set	λ	$C_{O3,out}$	β_{O3}	$C_{NO,out}$	$C_{NO2,out}$	β_{NO2}	J_{HONO}	C_{lim}	E_{NOY}/V	y-int	R^2
		Regression Coefficients for Oxidant Concentrations for R2 and R4										
C_{O3}	R2	0.79	1.2	-0.65	-0.16	-0.077	-0.0017	-0.0076	-0.061	0	-1.4	0.92
	R4	1.8	1.6	-0.32	-0.12	-0.039	-0.019	-0.0056	-0.024	-0.95	-0.70	0.95
C_{OH}	R2	0.61	0.99	-0.58	-0.10	-0.010	0.090	0.090	0.23	0	-16	0.92
	R4	0.30	0.74	-0.21	-0.050	-0.0057	0.28	0.44	-0.00061	-0.13	-14	0.72
C_{NO3}	R2	1.4	1.3	-0.72	-0.082	0.65	-0.59	-0.012	-0.76	0	-16	0.87
	R4	2.6	2.3	-0.44	-0.20	0.092	-0.62	-0.010	-0.36	-1.1	-15	0.92
		Regression Coefficients for VOC Oxidation Rates by Oxidant for R2 and R4										
VOC-ox(O_3)	R2	0.79	1.2	-0.65	-0.16	-0.077	-0.0032	-0.0073	0.82	0	-5.0	0.93
	R4	1.8	1.6	-0.32	-0.12	-0.040	-0.020	-0.0054	0.85	-0.95	-4.3	1.0
VOC-ox(OH)	R2	0.61	0.99	-0.58	-0.10	-0.011	0.086	0.090	0.77	0	-4.4	0.94
	R4	0.30	0.74	-0.20	-0.050	-0.0063	0.27	0.44	0.54	-0.13	-2.9	0.77
VOC-ox(NO_3)	R2	1.4	1.3	-0.72	-0.082	0.65	-0.59	-0.012	0.065	0	-8.2	0.86
	R4	2.6	2.3	-0.44	-0.20	0.091	-0.62	-0.0093	0.47	-1.1	-7.4	0.92

[a] Concentrations are units of ppb, oxidation rates in units of ppb/h