

Supplementary information for:

# Towards improved models for indoor air chemistry: a Monte Carlo simulation study

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VOC reaction	Rate coefficient (cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup> )	Individual variation (%)
Hexanal + OH	$2.88 \times 10^{-11}$	$\pm 19$
Heptanal + OH	$3.05 \times 10^{-11}$	$\pm 19$
Octanal + OH	$3.2 \times 10^{-11}$	$\pm 19$
Nonanal + OH	$3.6 \times 10^{-11}$	$\pm 19$
Decanal + OH	$3.6 \times 10^{-11}$	$\pm 19$
$\alpha$ -pinene + OH	$1.2 \times 10^{-11} \exp(440/T)$	$\pm 8$
$\beta$ -pinene + OH	$2.38 \times 10^{-11} \exp(357/T)$	$\pm 5$
Limonene + OH	$4.28 \times 10^{-11} \exp(401/T)$	$\pm 5$
Acetic acid + OH	$8.0 \times 10^{-13}$	$\pm 7$
Acetone + OH	$8.8 \times 10^{-12} \exp(-1320/T) + 1.7 \times 10^{-14} \exp(423/T)$	$\pm 8$
Methanol + OH	$2.85 \times 10^{-12} \exp(-345/T)$	$\pm 8$
Ethanol + OH	$3.0 \times 10^{-12} \exp(20/T)$	$\pm 6$
Isoprene + OH	$2.7 \times 10^{-11} \exp(390/T)$	$\pm 6$
Isopropanol + OH	$2.6 \times 10^{-12} \exp(200/T)$	$\pm 15$
Formaldehyde + OH	$5.4 \times 10^{-12} \exp(135/T)$	$\pm 8$
4-OPA + OH	$2.63 \times 10^{-11}$	$\pm 25$
$\alpha$ -pinene + O <sub>3</sub>	$6.3 \times 10^{-11} \exp(-580/T)$	$\pm 15$
$\beta$ -pinene + O <sub>3</sub>	$1.5 \times 10^{-17}$	$\pm 25$
Limonene + O <sub>3</sub>	$2.95 \times 10^{-15} \exp(783/T)$	$\pm 10$
Isoprene + O <sub>3</sub>	$1.03 \times 10^{-14} \exp(-1995/T)$	$\pm 6$

Table ST1: Key indoor VOC rate coefficients Bowman et al. (2003); Chacon-Madrid et al. (2010). T is temperature (K). Individual variation refers to the maximum and minimum values used for the individual variation analysis in section 2.3 according to their uncertainty from the International Union of Pure and Applied Chemistry (IUPAC) gas kinetics database Task Group on Atmospheric Chemical Kinetic Data Evaluation.

Parameter	Baseline value	Minimum value	Maximum value
Ozone deposition velocity hard furnishing (cm s <sup>-1</sup> )	0.005	0.003	0.0055
Ozone deposition velocity soft furnishing (cm s <sup>-1</sup> )	0.15	0.04	0.19
Ozone deposition velocity painted wall (cm s <sup>-1</sup> )	0.026	0.01	0.17
Ozone deposition velocity wooden floor (cm s <sup>-1</sup> )	0.069	0.014	0.142
Ozone deposition velocity linoleum (cm s <sup>-1</sup> )	0.007	0.004	0.0214
Ozone deposition velocity countertop (cm s <sup>-1</sup> )	0.136	0.129	0.149
Ozone deposition velocity skin (cm s <sup>-1</sup> )	0.285	0.2	0.403
Hexanal emission rate hard furniture (molecule cm <sup>-3</sup> s <sup>-1</sup> )	5.76×10 <sup>-6</sup>	4.61×10 <sup>-6</sup>	6.91×10 <sup>-6</sup>
Heptanal emission rate hard furniture (molecule cm <sup>-3</sup> s <sup>-1</sup> )	1.24×10 <sup>-7</sup>	9.95×10 <sup>-8</sup>	1.49×10 <sup>-7</sup>
Octanal emission rate hard furniture (molecule cm <sup>-3</sup> s <sup>-1</sup> )	1.20×10 <sup>-7</sup>	9.6×10 <sup>-8</sup>	1.44×10 <sup>-7</sup>
Nonanal emission rate hard furniture (molecule cm <sup>-3</sup> s <sup>-1</sup> )	2.69×10 <sup>-6</sup>	2.15×10 <sup>-6</sup>	3.23×10 <sup>-6</sup>
Hexanal yield soft furniture	0.026	0	0.08
Heptanal yield soft furniture	0.0073	0	0.04
Octanal yield soft furniture	0.0093	0	0.07
Nonanal yield soft furniture	0.06	0	0.14
Decanal yield soft furniture	0.0253	0	0.09
Octanal yield painted wall	0.01	0	0.03
Nonanal yield painted wall	0.133	0	0.34
Decanal yield painted wall	0.043	0	0.12
Hexanal emission rate wooden floor (molecule cm <sup>-3</sup> s <sup>-1</sup> )	1.35×10 <sup>-5</sup>	1.08×10 <sup>-5</sup>	1.62×10 <sup>-5</sup>
Heptanal emission rate wooden floor (molecule cm <sup>-3</sup> s <sup>-1</sup> )	2.91×10 <sup>-7</sup>	2.33×10 <sup>-7</sup>	3.49×10 <sup>-7</sup>
Octanal emission rate wooden floor (molecule cm <sup>-3</sup> s <sup>-1</sup> )	2.8×10 <sup>-7</sup>	2.24×10 <sup>-7</sup>	3.36×10 <sup>-7</sup>
Nonanal emission rate wooden floor (molecule cm <sup>-3</sup> s <sup>-1</sup> )	6.28×10 <sup>-6</sup>	5.02×10 <sup>-6</sup>	7.54×10 <sup>-6</sup>
Decanal emission rate wooden floor (molecule cm <sup>-3</sup> s <sup>-1</sup> )	1.65×10 <sup>-7</sup>	1.32×10 <sup>-7</sup>	1.98×10 <sup>-7</sup>
Hexanal yield linoleum	0.071	0	0.13
Heptanal yield linoleum	0.006	0	0.02
Octanal yield linoleum	0.014	0	0.05
Nonanal yield linoleum	0.131	0	0.25
Decanal yield linoleum	0.031	0	0.12
Hexanal yield countertop	0.078	0	0.17
Heptanal yield countertop	0.023	0	0.06
Octanal yield countertop	0.013	0	0.04
Nonanal yield countertop	0.257	0.01	0.62
Decanal yield countertop	0.033	0	0.16
Acetone yield skin	0.049	0.037	0.061
Formic acid yield skin	0.0085	0.0064	0.0106
Acetic acid yield skin	0.0065	0.0049	0.0081
4-oxopentanal yield skin	0.026	0.0195	0.033
Nonanal yield skin	0.018	0.014	0.023
Decanal yield skin	0.026	0.0195	0.033
Emission rate of acetone in breath (molecule cm <sup>-3</sup> s <sup>-1</sup> )	5.26×10 <sup>7</sup>	6.41×10 <sup>4</sup>	1×10 <sup>8</sup>
Emission rate of ethanol in breath (molecule cm <sup>-3</sup> s <sup>-1</sup> )	4.11×10 <sup>7</sup>	6.95×10 <sup>5</sup>	5.34×10 <sup>7</sup>
Emission rate of methanol in breath (molecule cm <sup>-3</sup> s <sup>-1</sup> )	1.76×10 <sup>7</sup>	6.95×10 <sup>4</sup>	1.07×10 <sup>8</sup>
Emission rate of isopropanol in breath (molecule cm <sup>-3</sup> s <sup>-1</sup> )	8.01×10 <sup>6</sup>	2.67×10 <sup>6</sup>	1.39×10 <sup>7</sup>
Emission rate of isoprene in breath (molecule cm <sup>-3</sup> s <sup>-1</sup> )	1.12×10 <sup>7</sup>	6.41×10 <sup>5</sup>	3.1×10 <sup>7</sup>
UV light transmission (%) (integrated over 300-400nm)	14	0	38
Visible light transmission (%) (integrated over 400-800nm)	49	41	57
Air exchange rate (h <sup>-1</sup> )	0.72	0.43	1.34
Internal temperature (K)	297.07	295.18	298.85
Relative humidity (%)	50.2	36.84	56.93
Total surface to volume ratio (cm <sup>-1</sup> )	0.0202	0.0182	0.0222
Soft furniture surface to volume ratio (cm <sup>-1</sup> )	0.00208	0.0019	0.0023
Painted wall surface to volume ratio (cm <sup>-1</sup> )	0.0118	0.0106	0.0130
Linoleum surface to volume ratio (cm <sup>-1</sup> )	0.00063	0.0006	0.0007
Countertop surface to volume ratio (cm <sup>-1</sup> )	0.00113	0.001	0.0012
Human body surface to volume ratio (cm <sup>-1</sup> )	0.000238	0.0002	0.0003
Outdoor concentrations of Ozone, NO <sub>x</sub> and particulate matter	Milan 2009 Terry et al. (2014)	0.5 × baseline	Milan 2003 heatwave Terry et al. (2014)

Table ST2: Minimum and maximum values of parameters used in the baseline model run in section 2.2 alongside those used for the individual sensitivity analysis in section 2.3.

Concentration distribution functions for all Monte Carlo simulations. In all cases the green line indicates the median concentration and the red lines show the minimum and maximum 95% confidence bounds with values given in Table 2. To create the probability density histograms the outputs were binned into 40 equally spaced bins between the maximum and minimum value output.

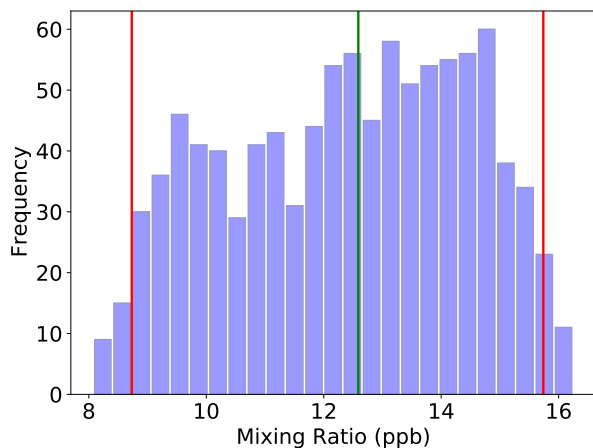


Figure S1: Ethanol

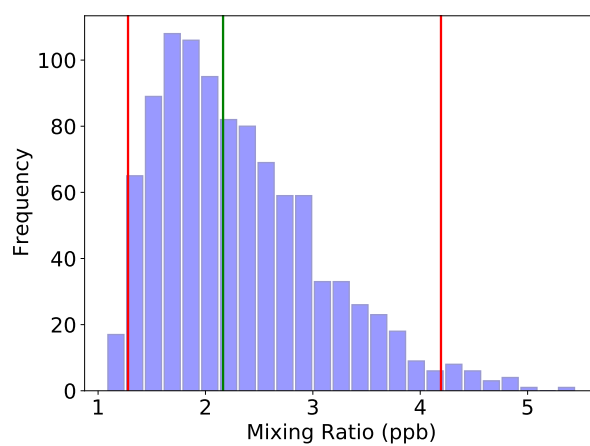


Figure S2: Hexanal

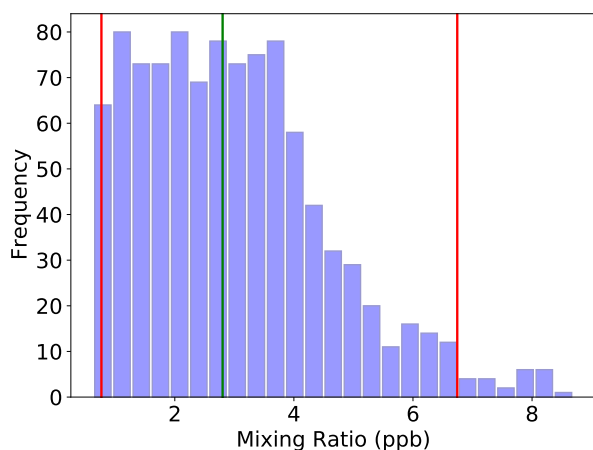


Figure S3: Isoprene

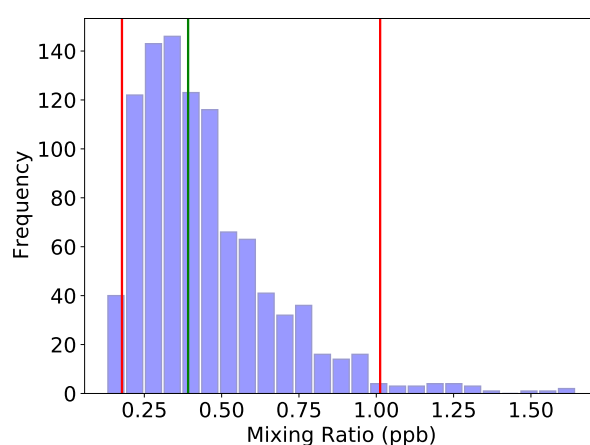


Figure S4: Heptanal

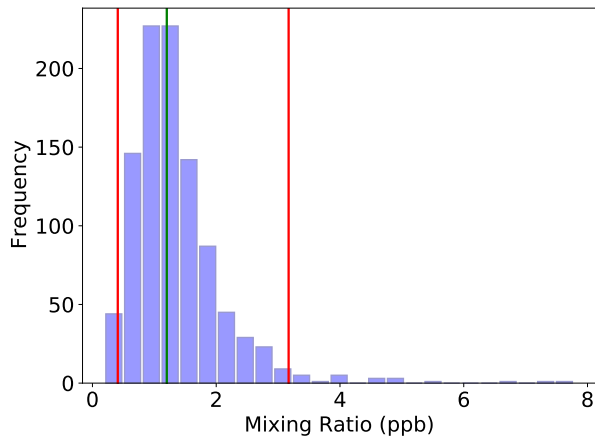


Figure S5: Octanal

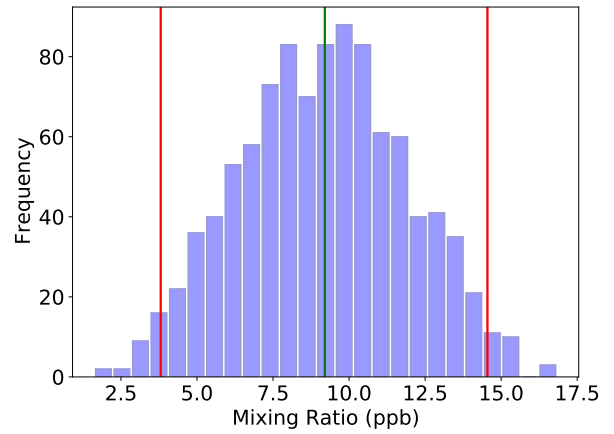


Figure S6: Nonanal

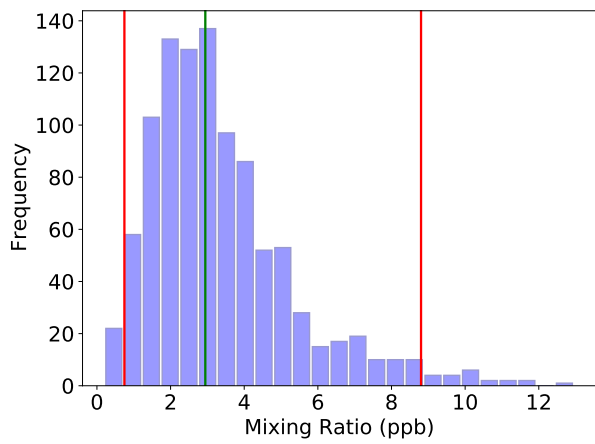


Figure S7: Decanal

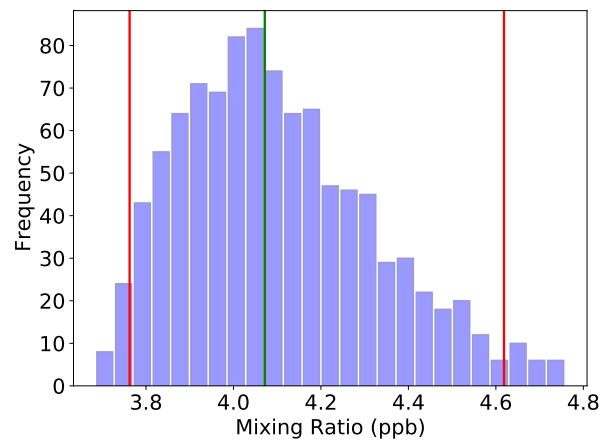


Figure S8: Acetaldehyde

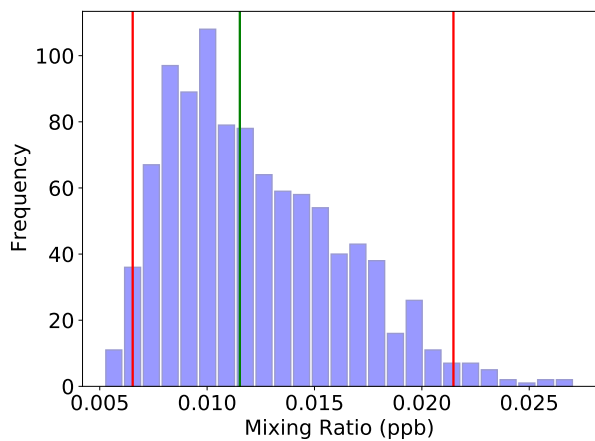


Figure S9: Acetic acid

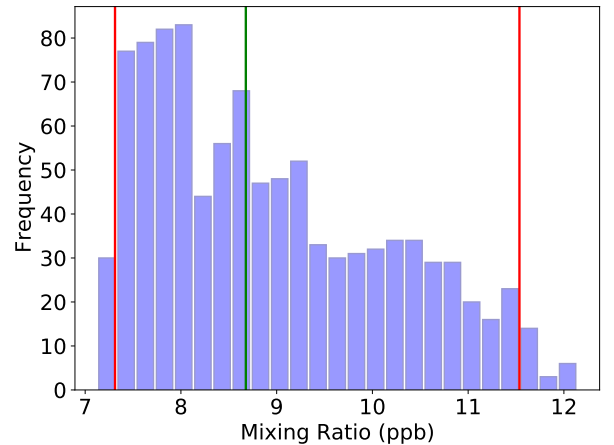


Figure S10: Acetone

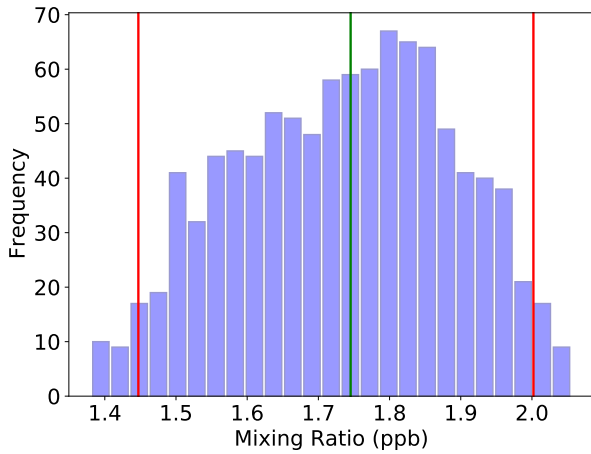


Figure S11: Methanol

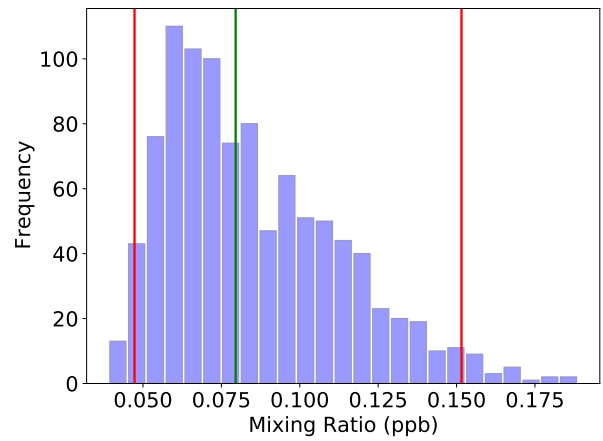


Figure S12: 4-oxopentanal

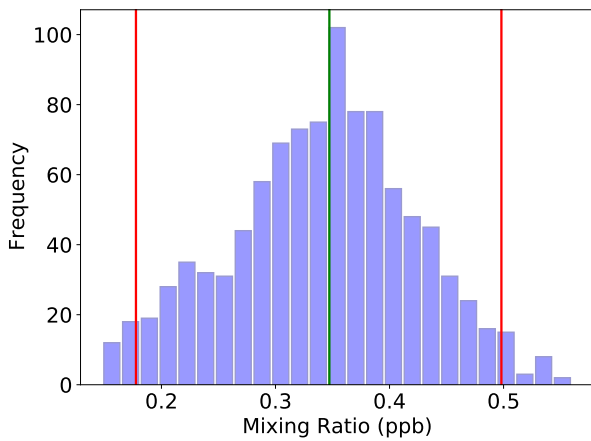


Figure S13: Glyoxal

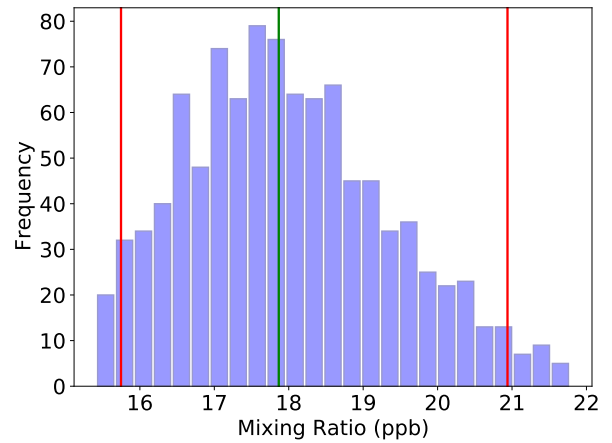


Figure S14: Formaldehyde

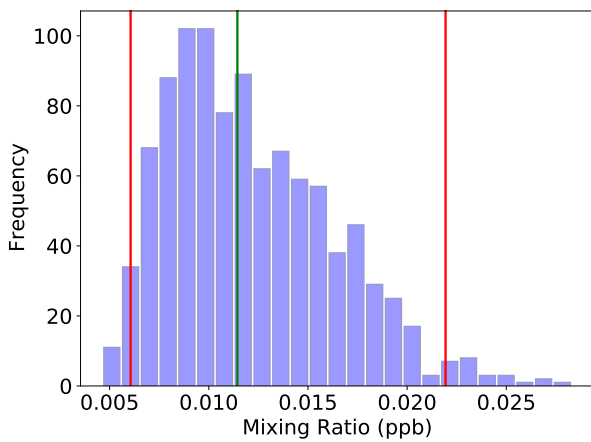


Figure S15: Formic acid

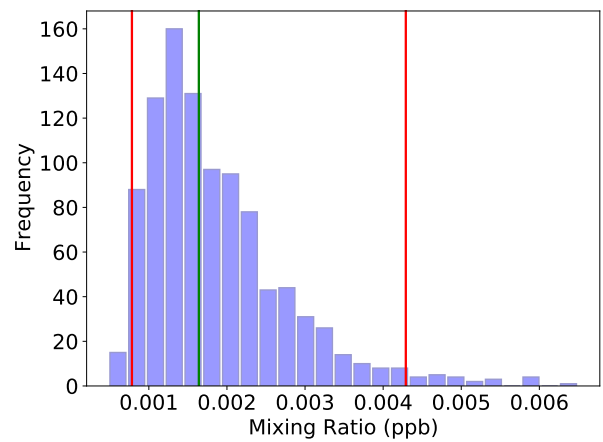


Figure S16: HO<sub>2</sub>

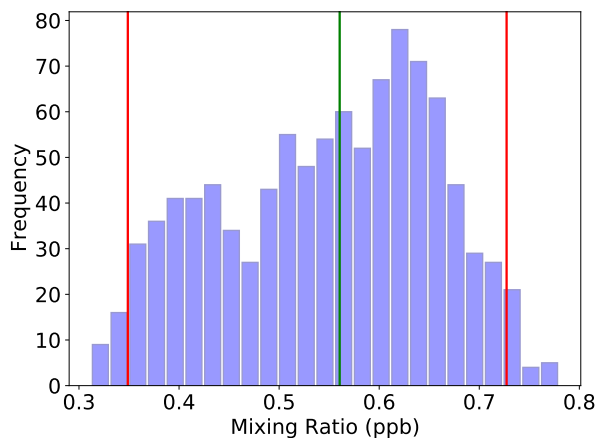


Figure S17: Nitrous acid

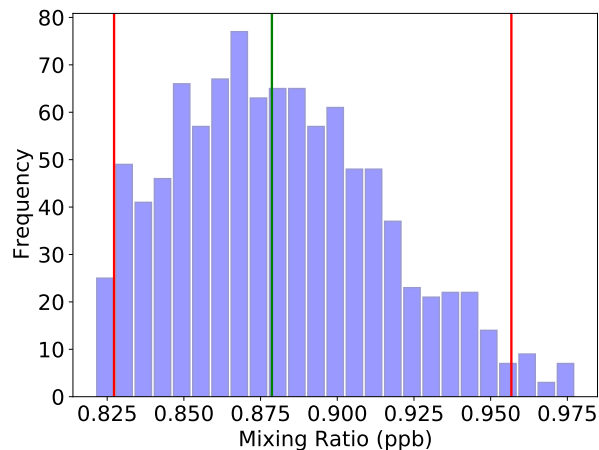


Figure S18: Isopropanol

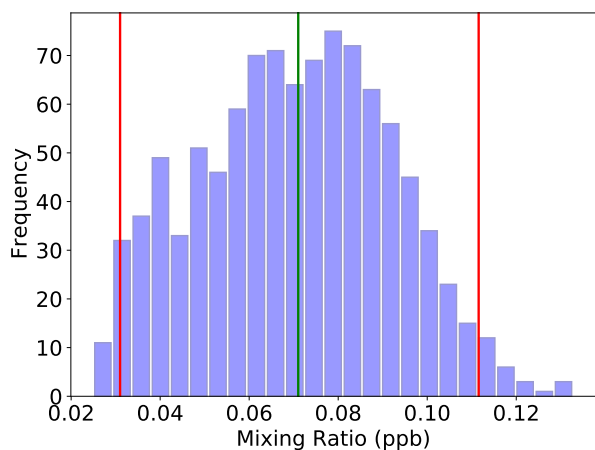


Figure S19: Methylglyoxal

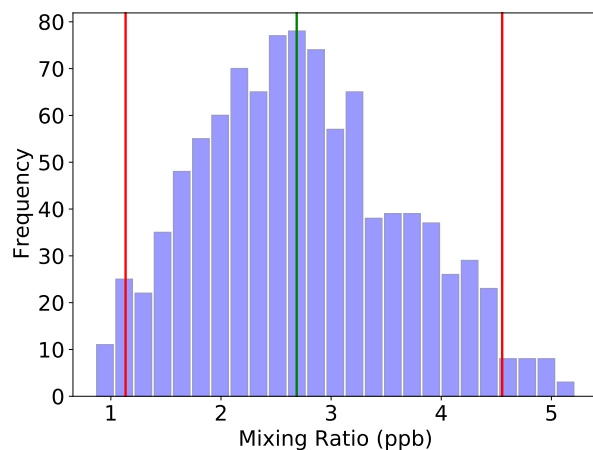


Figure S20: NO

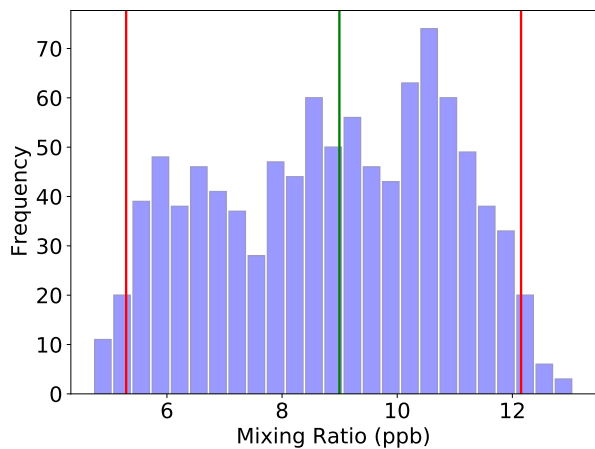


Figure S21: NO<sub>2</sub>

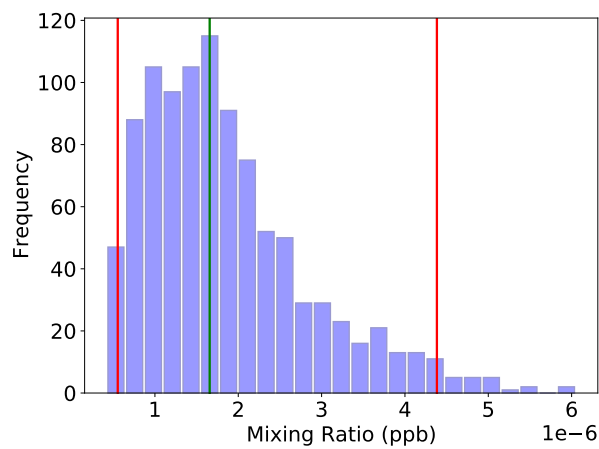


Figure S22: NO<sub>3</sub>

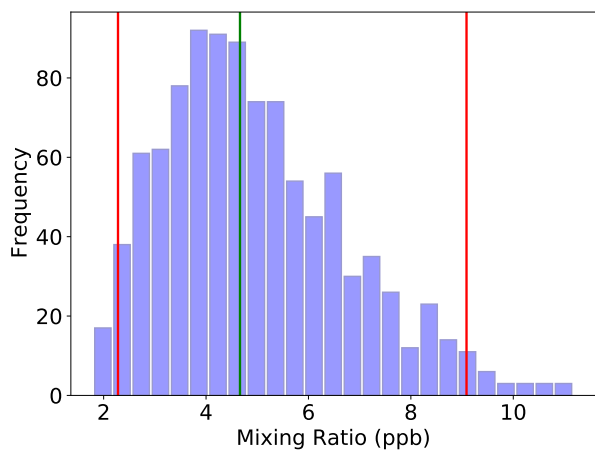


Figure S23: Ozone

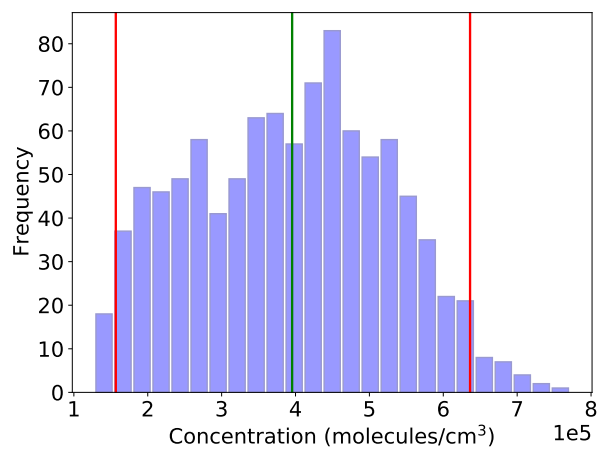


Figure S24: OH

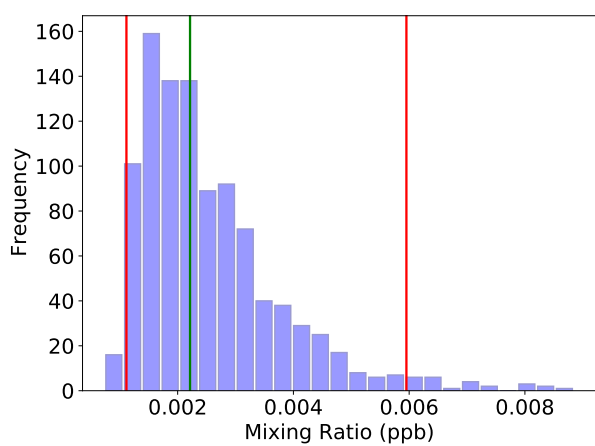


Figure S25: RO<sub>2</sub>

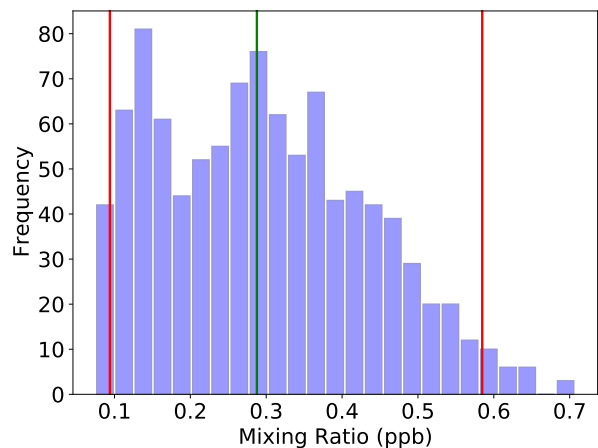


Figure S26: Total organic nitrates

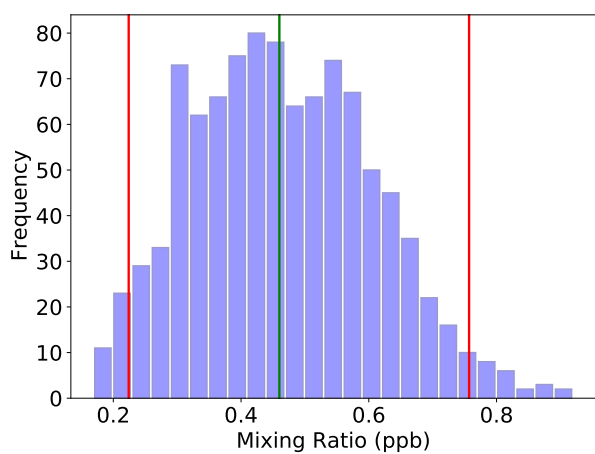


Figure S27: Total PAN species



	Air Exchange Rate (h <sup>-1</sup> )	UV light transmission (%)	Temperature (K)	Hexanal yield (soft furniture)	Heptanal yield (soft furniture)	Octanal yield (soft furniture)	Nonanal yield (soft furniture)	Decanal yield (soft furniture)	Octanal yield (painted walls)	Nonanal yield (painted walls)	Decanal yield (painted walls)	Soft furniture A/V (cm <sup>-2</sup> )	Painted wall A/V (cm <sup>-2</sup> )	Linoleum A/V (cm <sup>-2</sup> )	Countertop A/V (cm <sup>-2</sup> )	Human body A/V (cm <sup>-2</sup> )	Total A/V (cm <sup>-2</sup> )	O <sub>3</sub> soft furniture v <sub>d</sub> (cm s <sup>-1</sup> )	O <sub>3</sub> painted wall v <sub>d</sub> (cm s <sup>-1</sup> )	Isoprene emission rate (molecules cm <sup>-3</sup> s <sup>-1</sup> )
NO	1.2	37	298.5	0.065	0.015	0.0072	0.028	0.036	0.027	0.26	0.012	0.0022	0.012	0.00069	0.0011	0.00026	0.018	0.19	0.17	3e+07
Total organic nitrates	1.2	37	298.5	0.065	0.015	0.0072	0.028	0.036	0.027	0.26	0.012	0.0022	0.012	0.00069	0.0011	0.00026	0.018	0.19	0.17	3e+07
Hexanal	0.83	33	296.7	0.074	0.00049	0.013	0.01	0.028	0.012	0.32	0.074	0.002	0.012	0.00062	0.001	0.00023	0.018	0.18	0.041	1.9e+07
Formaldehyde	0.47	18	298.3	0.0085	0.034	0.051	0.13	0.026	0.0079	0.0065	0.12	0.002	0.011	0.00062	0.0011	0.00026	0.018	0.13	0.027	1.9e+07
Heptanal	0.87	21	297.5	0.0026	0.038	0.057	0.0092	0.034	0.02	0.12	0.08	0.0022	0.012	0.00061	0.001	0.00022	0.021	0.14	0.012	1.4e+07
NO <sub>3</sub>	1.2	18	298.4	0.039	0.036	0.045	0.017	0.018	0.018	0.074	0.094	0.0019	0.011	0.00062	0.0012	0.00023	0.021	0.05	0.016	1.3e+07
OH	1.1	38	297.2	0.069	0.024	0.043	0.01	0.051	0.012	0.19	0.11	0.0019	0.012	0.00062	0.0012	0.00026	0.022	0.039	0.019	1.5e+07
4-oxopentanal	0.83	23	298.6	0.029	0.023	0.0021	0.01	0.059	0.016	0.22	0.11	0.0022	0.013	0.00069	0.0011	0.00026	0.02	0.058	0.011	3e+07
Acetaldehyde	0.47	16	298.8	0.0042	0.03	0.00043	0.055	0.079	0.011	0.03	0.024	0.0019	0.011	0.00061	0.0011	0.00024	0.018	0.054	0.016	7.9e+06
O <sub>3</sub>	1.1	22	296.3	0.041	0.038	0.052	0.025	0.015	0.011	0.16	0.0076	0.0019	0.011	0.00064	0.0012	0.00024	0.019	0.054	0.011	2.9e+07
Glyoxal	1.1	22	296.3	0.041	0.038	0.052	0.025	0.015	0.011	0.16	0.0076	0.0019	0.011	0.00064	0.0012	0.00024	0.019	0.054	0.011	2.9e+07
Acetic acid	1.1	22	296.3	0.041	0.038	0.052	0.025	0.015	0.011	0.16	0.0076	0.0019	0.011	0.00064	0.0012	0.00024	0.019	0.054	0.011	2.9e+07
Formic acid	1.1	22	296.3	0.041	0.038	0.052	0.025	0.015	0.011	0.16	0.0076	0.0019	0.011	0.00064	0.0012	0.00024	0.019	0.054	0.011	2.9e+07
Nitrous acid	1.3	2.7	297.9	0.069	0.012	0.06	0.11	0.086	0.00034	0.13	0.098	0.0021	0.012	0.00066	0.0012	0.00022	0.019	0.1	0.023	2.8e+07
NO <sub>2</sub>	1.3	2.7	297.9	0.069	0.012	0.06	0.11	0.086	0.00034	0.13	0.098	0.0021	0.012	0.00066	0.0012	0.00022	0.019	0.1	0.023	2.8e+07
Methanol	1.3	32	297.2	0.0075	0.04	0.028	0.074	0.054	0.0016	0.24	0.098	0.0021	0.012	0.00067	0.001	0.00025	0.018	0.098	0.15	2.7e+06
Ethanol	1.3	32	297.2	0.0075	0.04	0.028	0.074	0.054	0.0016	0.24	0.098	0.0021	0.012	0.00067	0.001	0.00025	0.018	0.098	0.15	2.7e+06
Total PAN species	1.2	38	296.6	0.055	0.033	0.033	0.023	0.045	0.014	0.23	0.029	0.002	0.012	0.00057	0.0012	0.00024	0.018	0.15	0.026	2.3e+07
Acetone	0.44	13	297.4	0.077	0.018	0.066	0.073	0.0024	0.014	0.23	0.088	0.002	0.012	0.00067	0.0012	0.00023	0.018	0.19	0.023	6.3e+06
Decanal	1.3	33	295.4	0.014	0.016	0.017	0.13	0.086	0.0048	0.0057	0.096	0.0019	0.011	0.00063	0.001	0.00025	0.021	0.043	0.13	2.9e+06
Nonanal	1.1	37	297.3	0.028	0.019	0.024	0.0079	0.036	0.02	0.3	0.008	0.002	0.013	0.0006	0.001	0.00022	0.02	0.085	0.16	1e+07
Methylglyoxal	0.88	38	298.7	0.038	0.031	0.0042	0.1	0.015	0.023	0.23	0.034	0.0022	0.011	0.00062	0.0012	0.00023	0.019	0.088	0.019	2.2e+07
Isopropanol	0.45	11	296.9	0.0037	0.019	0.038	0.11	0.003	0.022	0.13	0.048	0.0022	0.012	0.00062	0.0011	0.00023	0.018	0.056	0.12	1e+07
Octanal	0.5	17	297.8	0.043	0.028	0.062	0.14	0.078	0.025	0.0058	0.0058	0.002	0.011	0.00061	0.0012	0.00024	0.021	0.066	0.14	1.2e+07
Isoprene	0.45	11	298.3	0.048	0.0088	0.067	0.034	0.053	0.023	0.093	0.057	0.0021	0.012	0.00062	0.001	0.00021	0.019	0.06	0.062	3.1e+07
RO <sub>2</sub>	0.48	36	298.7	0.049	0.034	0.047	0.027	0.043	0.027	0.28	0.079	0.0019	0.011	0.0006	0.0011	0.00025	0.021	0.05	0.032	3e+07
HO <sub>2</sub>	0.48	36	298.7	0.049	0.034	0.047	0.027	0.043	0.027	0.28	0.079	0.0019	0.011	0.0006	0.0011	0.00025	0.021	0.05	0.032	3e+07

Figure S28: The parameter values that corresponded to the maximum concentrations of individual chemical species which are grouped vertically by simulation run number. Red hues represent values near the maximum parameter value and blue hues represent values near the minimum parameter value. A/V corresponds to the area to volume ratio,  $v_d$  is the deposition velocity and isoprene emission comes from human breath.

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