Supporting Information

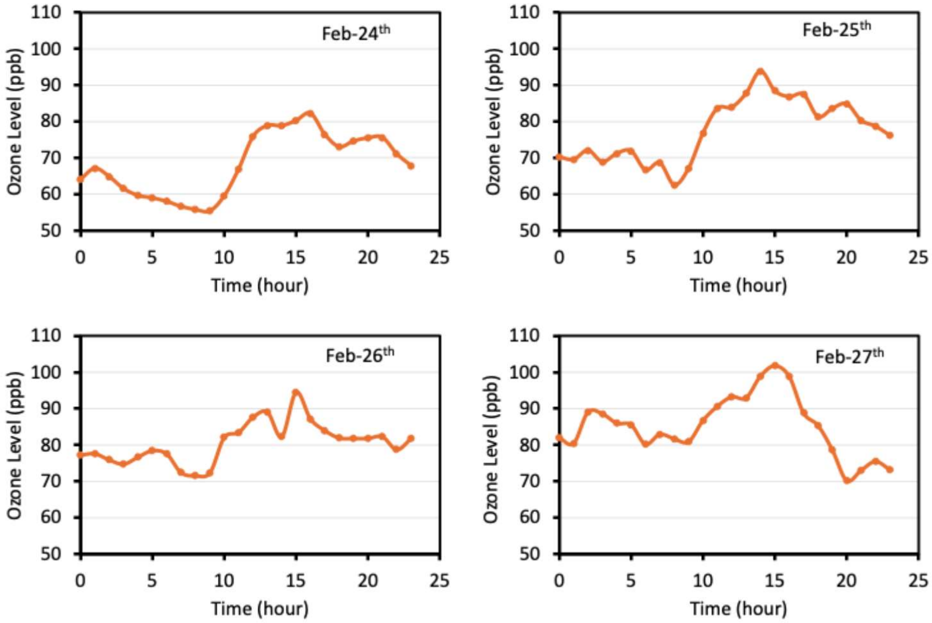

Figure S1: Diurnal variation of hourly average ozone levels during the simulation period (February 24–27, 2019).

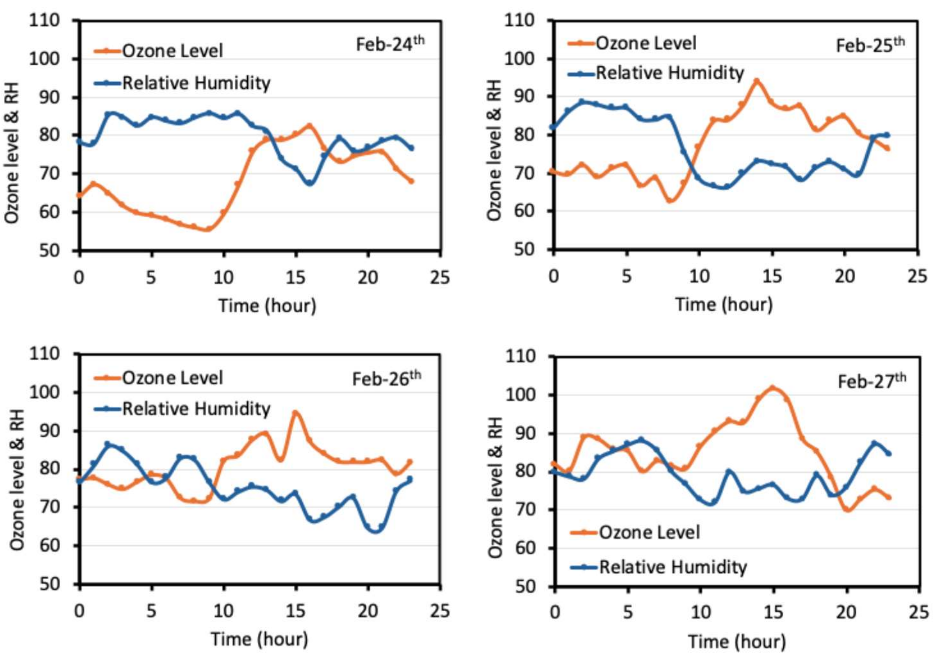

Figure S2: Diurnal trend of ozone level vs relative humidity (RH) during the simulation period.

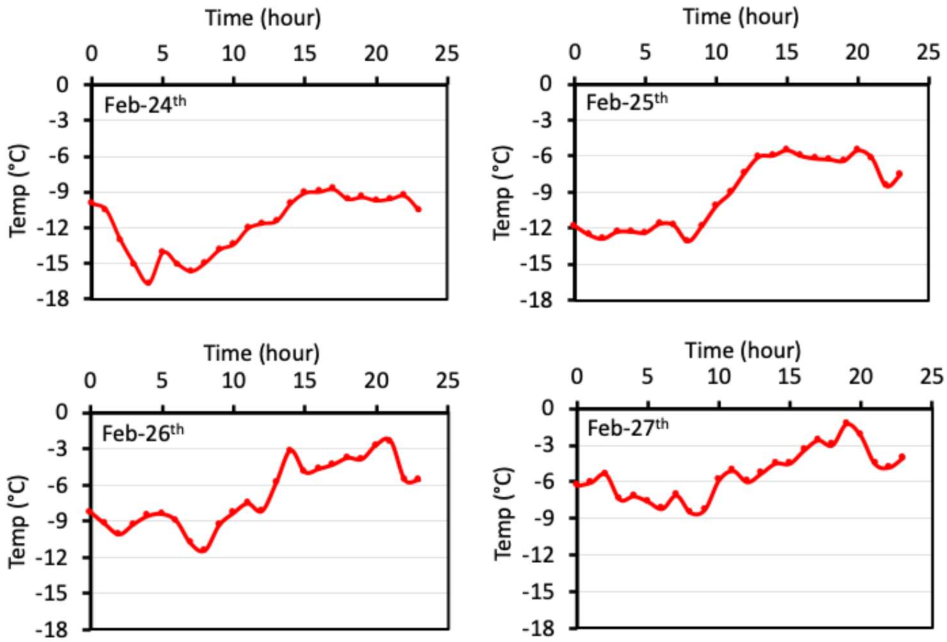

Figure S3: Diurnal trend of atmospheric temperature during the simulation period.

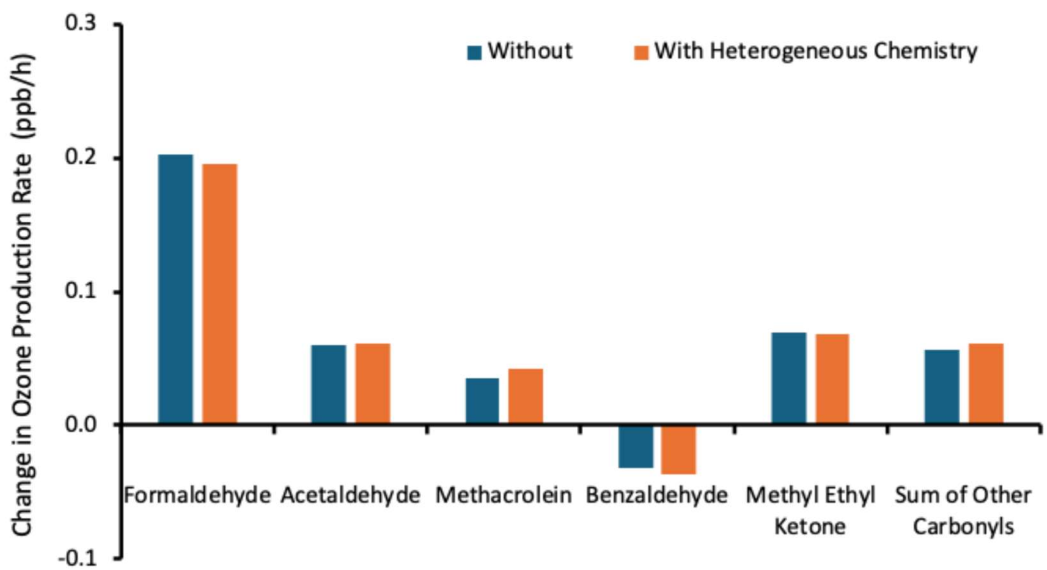

Figure S4: Impacts of specific carbonyl compounds on winter ozone production rates simulated by the F0AM box model with MCMv331, considering scenarios with and without heterogeneous chemistry. Bars represent the changes in ozone production rate resulting from a 50% increase in the mixing ratio of each NMOC group.

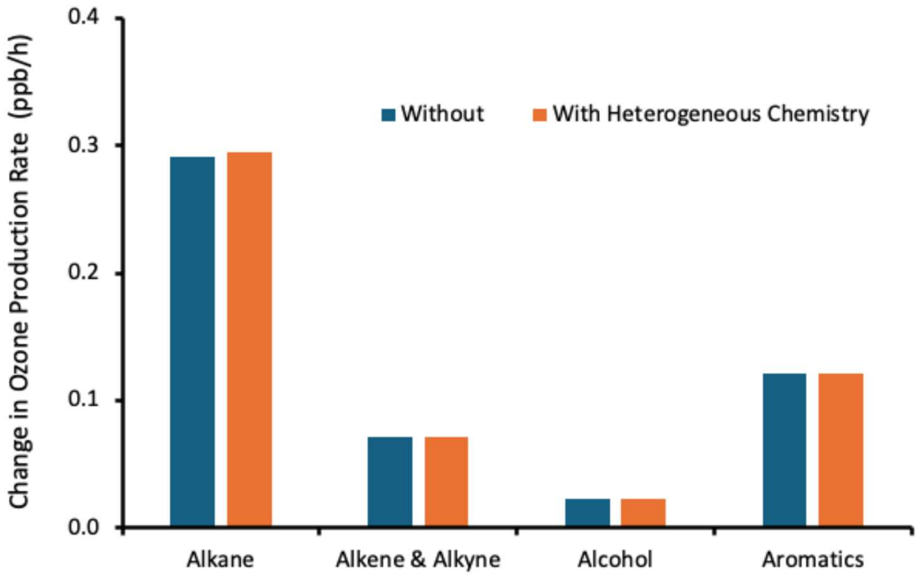

Figure S5: Impacts of the changes in NMOC precursor groups on winter O_3 production rates simulated by the F0AM box model with MCMv331, considering scenarios with and without heterogeneous chemistry. Bars represent the changes in O_3 production rate resulting from a 50% increase in the mixing ratio of each NMOC group.

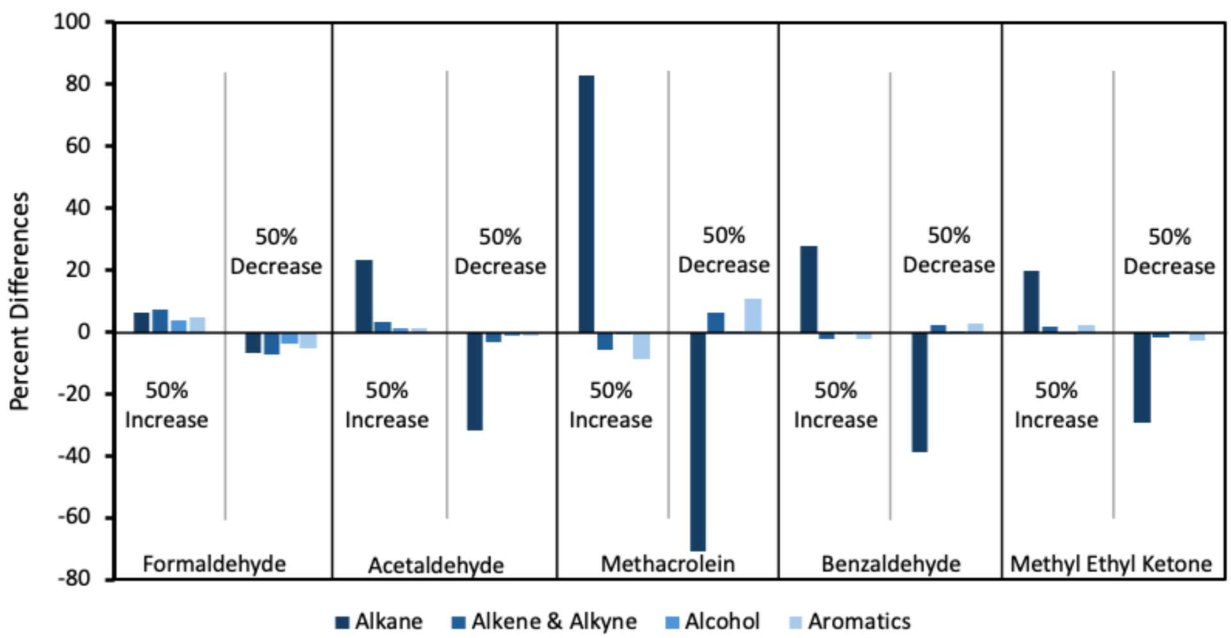

Figure S6: Sensitivity of carbonyl compounds to changes in NMOC precursor groups (MCMv331 Output). Bars represent the changes in carbonyl mixing ratios resulting from a ±50% change in the mixing ratio of each NMOC group.

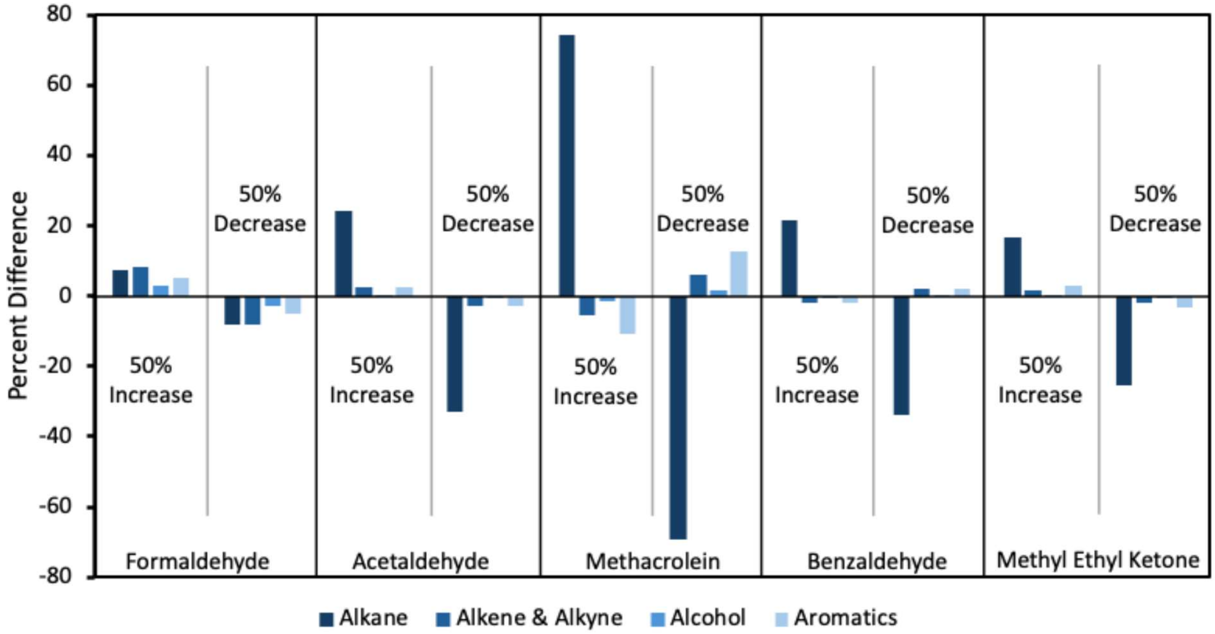

Figure S7: Sensitivity of carbonyl compounds to changes in NMOC precursor groups (SAPRC07 Output). Bars represent the changes in carbonyl mixing ratios resulting from a ±50% change in the mixing ratio of each NMOC group.

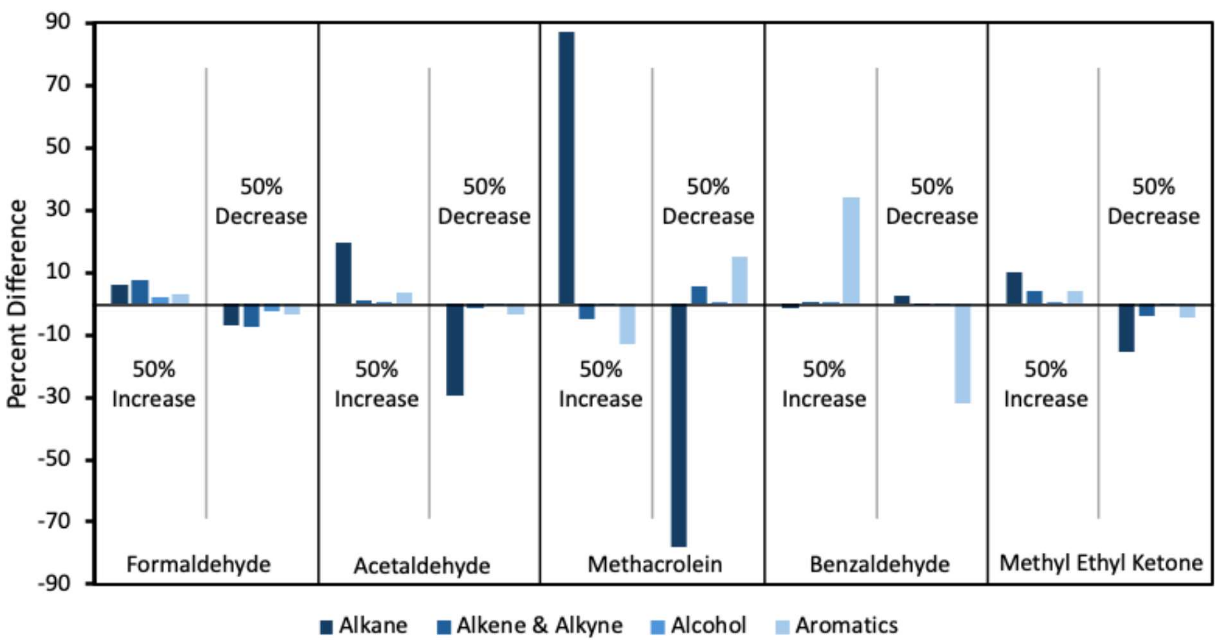

Figure S8: Sensitivity of carbonyl compounds to changes in NMOC precursor groups (RACM2 Output). Bars represent the changes in carbonyl mixing ratios resulting from a ±50% change in the mixing ratio of each NMOC group.

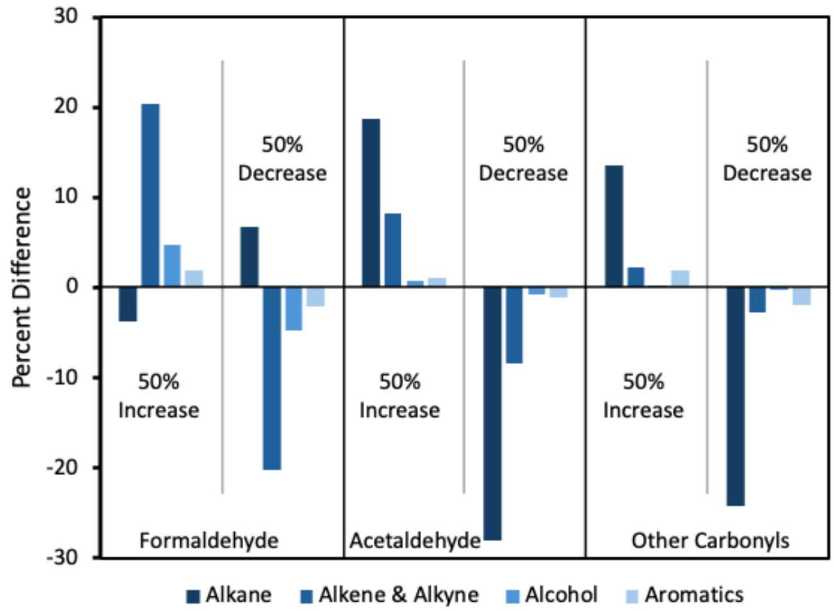

Figure S9: Sensitivity of carbonyl compounds to changes in NMOC precursor groups (CB6 Output). Bars represent the changes in carbonyl mixing ratios resulting from a ±50% change in the mixing ratio of each NMOC group.

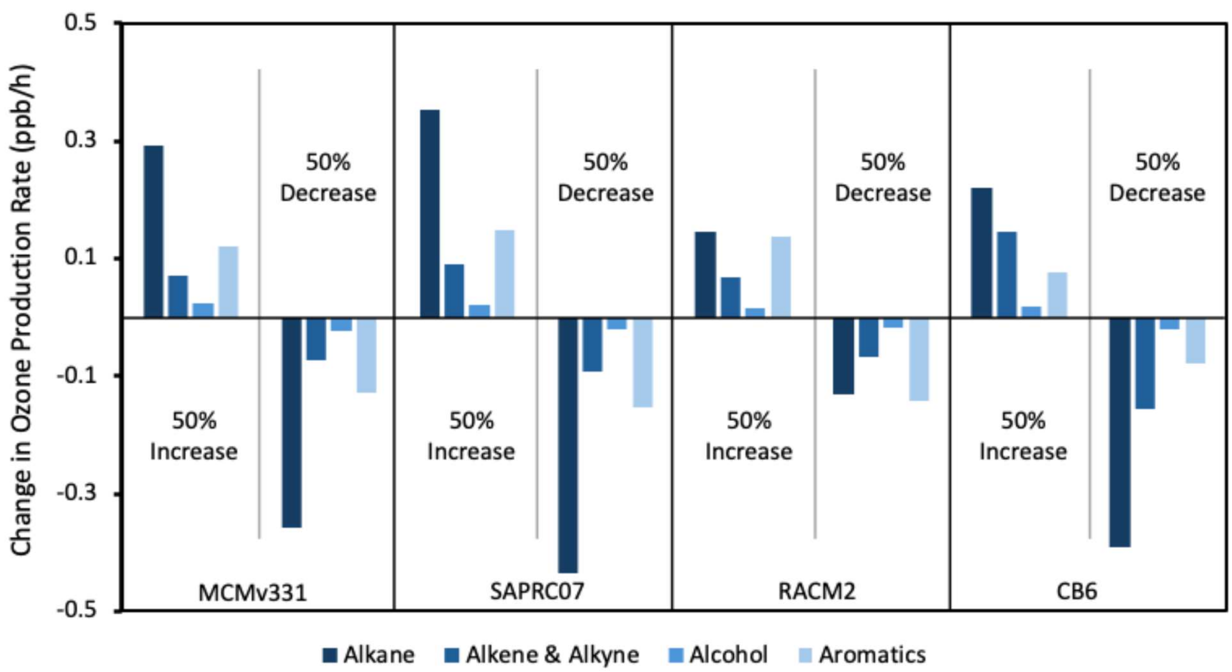

Figure S10: Sensitivity of O_3 production rate to changes in NMOC precursor groups within different chemical mechanisms (MCMv331, SAPCR07, RACM2 & CB6). The bars represent the changes in O_3 production rate due to increase & decrease in NMOC mixing ratio of 50%.

Table S1: Initial and maximum mixing ratio at day 4th of carbonyl species with their emission flux according to MCMv331.

Carbonyl Species	Initial Mixing Ratio (ppb)	Emission Flux (Molecules cm^{-2} s^{-1})	Max Mixing Ratio (ppb) at day four.
Formaldehyde	0.9	0.0	1.4
Acetaldehyde	0.6	0.0	2.2
Propionaldehyde	0.0	0.0	0.6
Butyraldehyde	0.4	0.2	0.5
Valeraldehyde	0.0	0.0	0.0
Acrolein	0.4	0.2	0.6
Methacrolein	0.2	0.2	0.4
Crotonaldehyde	0.0	0.0	0.0
Benzaldehyde	1.6	0.1	1.8
Acetone	0.7	0.0	4.7
Methyl ethyl ketone	0.2	0.0	1.6
Cyclohexanone	0.0	0.0	0.3

Table S2: Influence of ±50% changes in the initial mixing ratios of non-methane organic compounds (NMOC) on ozone (O_3) production rates (MCMv331 Output), with ambient mixing ratios for relative importance.

NMOC Group	Species	ΔO_3 Rate (+50% in NMOC) (ppb/h)	ΔO_3 Rate (-50% in NMOC) (ppb/h)	Mixing Ratio (ppb)
Alkane	Methane	0.043	-0.044	4920.0
	Ethane	0.021	-0.022	123.0
	Propane	0.027	-0.027	63.0
	n-Butane	0.053	-0.055	25.0
	Isobutane	0.084	-0.088	15.0
	n-Pentane	0.022	-0.022	10.0
	Isopentane	0.048	-0.050	11.0
	n-Hexane	0.001	0.000	4.0
	2-Methylpentane	0.017	-0.017	3.0
	3-Methylpentane	0.013	-0.014	2.0
	2,2-Dimethylbutane	0.001	-0.001	0.3
	2,3-Dimethylbutane	0.008	-0.008	1.6
	n-Heptane	-0.007	0.008	1.9
	2-Methylhexane	0.001	-0.001	0.8
	3-Methylhexane	0.001	-0.001	1.2
	n-Octane	-0.007	0.007	0.8

	n-Nonane	-0.003	0.003	0.2
	n-Decane	-0.004	0.004	0.2
	Cyclohexane	0.000	0.000	1.8
Alkenes & alkyne	Ethylene	0.045	-0.046	1.1
	Propylene	0.023	-0.023	0.1
	Acetylene	0.004	-0.004	1.8
Alcohol	Methanol	0.016	-0.016	10.0
	Ethanol	0.001	-0.001	0.3
	Isopropyl alcohol	0.006	-0.006	2.3
Aromatics	Benzene	0.007	-0.007	1.2
	Toluene	0.043	-0.044	1.2
	o-Xylene	0.009	-0.010	0.1
	m-Xylene	0.031	-0.031	0.2
	p-Xylene	0.011	-0.011	0.1
	Ethylbenzene	0.004	-0.004	0.1
	1,2,3-Trimethylbenzene	0.020	-0.020	0.1

Table S3: Percent change in formaldehyde (HCHO) formation in response to ±50% changes in the initial mixing ratios of NMOC (MCMv331 Output), with ambient mixing ratios for relative importance.

NMOC Group	Species	ΔHCHO Formation (%; +50% NMOC)	ΔHCHO Formation (%; -50% NMOC)	Mixing Ratio (ppb)
Alkane	Methane	6.168	-6.141	4920.0
	Ethane	0.743	-0.759	123.0
	Propane	-2.046	2.257	63.0
	n-Butane	-0.700	0.802	25.0
	Isobutane	7.440	-7.543	15.0
	n-Pentane	-0.339	0.369	10.0
	Isopentane	0.169	-0.158	11.0
	n-Hexane	-0.760	0.822	4.0
	2-Methylpentane	-0.300	0.323	3.0
	3-Methylpentane	0.161	-0.159	2.0
	2,2-Dimethylbutane	0.019	-0.016	0.3
	2,3-Dimethylbutane	-0.433	0.445	1.6
	n-Heptane	-0.806	0.856	1.9
	2-Methylhexane	-0.218	0.226	0.8
	3-Methylhexane	-0.416	0.433	1.2
	n-Octane	-0.582	0.603	0.8
	n-Nonane	-0.179	0.183	0.2
	n-Decane	-0.205	0.210	0.2
	Cyclohexane	-0.712	0.740	1.8
Alkenes & alkyne	Ethylene	4.604	-4.568	1.1
	Propylene	2.486	-2.471	0.1

	Acetylene	0.137	-0.134	1.8
Alcohol	Methanol	3.096	-3.076	10.0
	Ethanol	0.066	-0.065	0.3
	Isopropyl alcohol	0.550	-0.553	2.3
Aromatics	Benzene	0.177	-0.174	1.2
	Toluene	1.648	-1.658	1.2
	o-Xylene	0.413	-0.411	0.1
	m-Xylene	1.232	-1.237	0.2
	p-Xylene	0.428	-0.425	0.1
	Ethylbenzene	0.089	-0.085	0.1
	1,2,3-Trimethylbenzene	1.020	-1.024	0.1

Table S4: Percent change in acetaldehyde (CH_3CHO) formation in response to ±50% changes in the initial mixing ratios of NMOC (MCMv331 Output), with ambient mixing ratios for relative importance.

NMOC Group	Species	ΔCH_3CHO Formation (%; +50% NMOC)	ΔCH_3CHO Formation (%; -50% NMOC)	Mixing Ratio (ppb)
Alkane	Methane	0.072	-0.089	4920.0
	Ethane	10.535	-10.688	123.0
	Propane	0.315	-0.329	63.0
	n-Butane	3.757	-3.886	25.0
	Isobutane	-0.208	0.154	15.0
	n-Pentane	-0.100	0.114	10.0
	Isopentane	11.086	-11.490	11.0
	n-Hexane	-0.072	0.060	4.0
	2-Methylpentane	-0.250	0.262	3.0
	3-Methylpentane	2.872	-2.907	2.0
	2,2-Dimethylbutane	0.016	-0.017	0.3
	2,3-Dimethylbutane	-0.373	0.378	1.6
	n-Heptane	-0.143	0.133	1.9
	2-Methylhexane	-0.364	0.369	0.8
	3-Methylhexane	0.246	-0.247	1.2
	n-Octane	-0.132	0.131	0.8
	n-Nonane	-0.089	0.089	0.2
	n-Decane	-0.123	0.124	0.2
	Cyclohexane	-0.664	0.679	1.8
Alkenes & alkyne	Ethylene	0.359	-0.379	1.1
	Propylene	2.880	-2.873	0.1
	Acetylene	0.062	-0.063	1.8

Alcohol	Methanol	0.115	-0.118	10.0
	Ethanol	0.510	-0.511	0.3
	Isopropyl alcohol	0.743	-0.748	2.3
Aromatics	Benzene	0.060	-0.060	1.2
	Toluene	0.312	-0.341	1.2
	o-Xylene	0.081	-0.083	0.1
	m-Xylene	0.277	-0.290	0.2
	p-Xylene	0.117	-0.118	0.1
	Ethylbenzene	0.134	-0.134	0.1
	1,2,3-Trimethylbenzene	0.234	-0.239	0.1

Table S5: Percent change in methacrolein (MACR) formation in response to ±50% changes in the initial mixing ratios of NMOC (MCMv331 Output), with ambient mixing ratios for relative importance.

NMOC Group	Species	ΔMACR Formation (%; +50% NMOC)	ΔMACR Formation (%; -50% NMOC)	Mixing Ratio (ppb)
Alkane	Methane	-1.791	1.900	4920.0
	Ethane	3.490	-3.490	123.0
	Propane	10.293	-10.050	63.0
	n-Butane	10.134	-9.941	25.0
	Isobutane	-1.130	1.498	15.0
	n-Pentane	9.632	-9.439	10.0
	Isopentane	9.322	-9.180	11.0
	n-Hexane	8.385	-8.226	4.0
	2-Methylpentane	4.594	-4.577	3.0
	3-Methylpentane	2.971	-2.946	2.0
	2,2-Dimethylbutane	0.092	-0.092	0.3
	2,3-Dimethylbutane	2.209	-2.201	1.6
	n-Heptane	6.485	-6.360	1.9
	2-Methylhexane	2.192	-2.184	0.8
	3-Methylhexane	3.824	-3.791	1.2
	n-Octane	3.715	-3.674	0.8
	n-Nonane	1.197	-1.197	0.2
	n-Decane	1.406	-1.389	0.2
	Cyclohexane	3.582	-3.560	1.8
Alkenes & alkyne	Ethylene	-3.029	3.213	1.1
	Propylene	-2.444	2.544	0.1
	Acetylene	-0.485	0.485	1.8

Alcohol	Methanol	-1.247	1.272	10.0
	Ethanol	0.109	-0.117	0.3
	Isopropyl alcohol	0.921	-0.921	2.3
Aromatics	Benzene	-0.527	0.527	1.2
	Toluene	-3.414	3.665	1.2
	o-Xylene	-0.762	0.770	0.1
	m-Xylene	-2.444	2.586	0.2
	p-Xylene	-0.962	0.979	0.1
	Ethylbenzene	-0.351	0.343	0.1
	1,2,3-Trimethylbenzene	-1.096	1.146	0.1

Table S6: Percent change in benzaldehyde (Benzal) formation in response to ±50% changes in the initial mixing ratios of NMOC (MCMv331 Output), with ambient mixing ratios for relative importance.

NMOC Group	Species	ΔMACR Formation (%; +50% NMOC)	ΔMACR Formation (%; -50% NMOC)	Mixing Ratio (ppb)
Alkane	Methane	-0.651	0.685	4920.0
	Ethane	1.411	-1.437	123.0
	Propane	4.036	-4.186	63.0
	n-Butane	3.987	-4.148	25.0
	Isobutane	-0.319	0.461	15.0
	n-Pentane	3.765	-3.905	10.0
	Isopentane	3.689	-3.835	11.0
	n-Hexane	3.260	-3.361	4.0
	2-Methylpentane	1.835	-1.878	3.0
	3-Methylpentane	1.188	-1.202	2.0
	2,2-Dimethylbutane	0.038	-0.038	0.3
	2,3-Dimethylbutane	0.887	-0.893	1.6
	n-Heptane	2.524	-2.574	1.9
	2-Methylhexane	0.870	-0.875	0.8
	3-Methylhexane	1.503	-1.530	1.2
	n-Octane	1.450	-1.467	0.8
	n-Nonane	0.474	-0.475	0.2
	n-Decane	0.551	-0.553	0.2
	Cyclohexane	1.417	-1.440	1.8
Alkenes & alkyne	Ethylene	-1.163	1.207	1.1
	Propylene	-0.945	0.968	0.1
	Acetylene	-0.189	0.187	1.8

Alcohol	Methanol	-0.474	0.479	10.0
	Ethanol	0.044	-0.047	0.3
	Isopropyl alcohol	0.375	-0.379	2.3
Aromatics	Benzene	-0.196	0.195	1.2
	Toluene	-0.090	0.167	1.2
	o-Xylene	-0.287	0.291	0.1
	m-Xylene	-0.930	0.964	0.2
	p-Xylene	-0.367	0.370	0.1
	Ethylbenzene	-0.080	0.080	0.1
	1,2,3-Trimethylbenzene	-0.407	0.419	0.1

Table S7: Percent change in methyl ethyl ketone (MEK) formation in response to ±50% changes in the initial mixing ratios of NMOC (MCMv331 Output), with ambient mixing ratios for relative importance.

NMOC Group	Species	ΔMEK Formation (%; +50% NMOC)	ΔMEK Formation (%; -50% NMOC)	Mixing Ratio (ppb)
Alkane	Methane	0.424	-0.447	4920.0
	Ethane	-1.183	1.225	123.0
	Propane	-3.216	3.487	63.0
	n-Butane	37.599	-40.113	25.0
	Isobutane	0.091	-0.198	15.0
	n-Pentane	-2.915	3.154	10.0
	Isopentane	-2.050	2.234	11.0
	n-Hexane	-2.498	2.671	4.0
	2-Methylpentane	-1.448	1.510	3.0
	3-Methylpentane	5.227	-5.322	2.0
	2,2-Dimethylbutane	-0.027	0.028	0.3
	2,3-Dimethylbutane	-0.695	0.706	1.6
	n-Heptane	-1.913	2.006	1.9
	2-Methylhexane	-0.660	0.671	0.8
	3-Methylhexane	-1.089	1.122	1.2
	n-Octane	-1.103	1.133	0.8
	n-Nonane	-0.363	0.368	0.2
	n-Decane	-0.421	0.430	0.2
	Cyclohexane	-1.135	1.170	1.8
Alkenes & alkyne	Ethylene	0.892	-0.918	1.1
	Propylene	0.674	-0.686	0.1
	Acetylene	0.139	-0.137	1.8

Alcohol	Methanol	0.334	-0.336	10.0
	Ethanol	-0.039	0.040	0.3
	Isopropyl alcohol	-0.322	0.325	2.3
Aromatics	Benzene	0.144	-0.145	1.2
	Toluene	0.852	-0.896	1.2
	o-Xylene	0.193	-0.194	0.1
	m-Xylene	0.627	-0.648	0.2
	p-Xylene	0.264	-0.265	0.1
	Ethylbenzene	0.091	-0.091	0.1
	1,2,3-Trimethylbenzene	0.261	-0.270	0.1

Table S8.1: Ozone Production and Loss Budget on Day 4 (MCMv331 Output).

Top 5 Reactions Contributing to Ozone Production			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Production (%)
1	$O \rightarrow O_3$	1.25×10^{3}	100
2	$CH_3CO_3 + HO_2 \rightarrow$ Products + O_3	2.82×10^{-3}	2.26×10^{-4}
3	$C_6H5CO_3 + HO_2 \rightarrow$ Products + O_3	9.91×10^{-4}	7.93×10^{-5}
4	$C_2H5CO_3 + HO_2 \rightarrow$ Products + O_3	6.90×10^{-4}	5.52×10^{-5}
5	$C3H7CO_3 + HO_2 \rightarrow$ Products + O_3	4.16×10^{-4}	3.33×10^{-5}
	Total Production	= 1.25×10^{3} molecules cm^{-3}	
Top 5 Reactions Contributing to Ozone Loss			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Loss (%)
1	$O_3 + h\nu \rightarrow O$	9.29×10^{2}	75.9
2	$NO + O_3 \rightarrow$ Products	2.45×10^{2}	20.0
3	$O_3 + h\nu \rightarrow O^1D$	4.22×10^{1}	3.45
4	$NO_2 + O_3 \rightarrow$ Products	3.33	0.272
5	$C_6H_5O + O_3 \rightarrow$ Products	2.31	0.189
	Total Loss	= 1.22×10^{3} molecules cm^{-3}	

Table S8.2: Ozone Production and Loss Budget on Day 4 (SAPRC07 Output).

Top 5 Reactions Contributing to Ozone Production			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Production (%)
1	$O^3P + O_2 + M \rightarrow O_3$	1.28×10^{3}	100
2	$MECO_3$ (Methyl ethyl peroxy radical) + $HO_2 \rightarrow$ Products + O_3	6.89×10^{-3}	5.39×10^{-4}
3	RCO_3 (Acyl peroxy radical)+ $HO_2 \rightarrow$ Products + O_3	2.05×10^{-3}	1.60×10^{-4}

4	$BZCO_3$ (Benzoyl peroxy radical) + HO_2 → Products + O_3	1.05×10^{-3}	8.22×10^{-5}
5	$MACO_3$ (Methacryloyl peroxy radical) + HO_2 → Products + O_3	7.13×10^{-4}	5.58×10^{-5}
	Total Production	= 1.28×10^3 molecules cm^{-3}	
Top 5 Reactions Contributing to Ozone Loss			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Loss (%)
1	O_3 + hν → O^3P	9.52×10^2	76.2
2	NO + O_3 → Products	2.50×10^2	20.0
3	O_3 + hν → O^1D	4.32×10^1	3.46
4	NO_2+ O_3 → Products	3.43	0.275
5	HO_2 + O_3 → Products	0.940	0.0752
	Total Loss	= 1.25×10^3 molecules cm^{-3}	

Table S8.3: Ozone Production and Loss Budget on Day 4 (RACM2 Output).

Reaction Contributing to Ozone Production			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Production (%)
1	O^3P + O_2 → O_3	1.17×10^3	100
	Total Production	= 1.17×10^3 molecules cm^{-3}	
Top 5 Reactions Contributing to Ozone Loss			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Loss (%)
1	O_3 → O^3P + O_2	8.62×10^2	74.9
2	O_3 + NO → Products	2.45×10^2	21.3
3	O_3 → Products	3.91×10^1	3.40
4	NO_2 + O_3 → Products	3.07	0.267
5	O_3 + HO_2 → Products	0.705	0.0613
	Total Loss	= 1.15×10^3 molecules cm^{-3}	

Table S8.4: Ozone Production and Loss Budget on Day 4 (CB6 Output).

Reactions Contributing to Ozone Production			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Production (%)
1	O^3P → O_3	1.38×10^3	100
2	C_3O_2 + HO_2 → Products + O_3	6.07×10^{-3}	4.40×10^{-4}
3	CXO_3 (Acyl peroxy radical) + HO_2 → Products + O_3	3.78×10^{-3}	2.74×10^{-4}
4	OPO_3 (Glyoxyl peroxyacyl radical) + HO_2 → Products + O_3	1.09×10^{-3}	7.87×10^{-5}
	Total Production	= 1.38×10^3 molecules cm^{-3}	

Top 5 Reactions Contributing to Ozone Loss			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Loss (%)
1	$O_3 \rightarrow O^3P$	1.05×10^3	77.7
2	$NO + O_3 \rightarrow$ Products	2.47×10^2	18.3
3	$O_3 \rightarrow O^1D$	4.75×10^1	3.53
4	$NO_2 + O_3 \rightarrow$ Products	3.78	0.280
5	$HO_2 + O_3 \rightarrow$ Products	1.58	0.117
	Total Loss	= 1.35×10^3 molecules cm^{-3}	

Table S9.1: Hydrogen oxide radicals (HOx) Production and Loss Budget on Day 4 (MCMv331 Output)

Top 5 Reactions Contributing to HOx Production			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Production (%)
1	$HO_2NO_2 \rightarrow HO_2$ + Products	4.92	23.2
2	$CH_3O \rightarrow HO_2$ + Products	1.83	8.62
3	$O^1D \rightarrow OH + OH$	1.83	8.62
4	$HCHO + h\nu \rightarrow HO_2 + HO_2 +$ Products	1.69	7.99
5	$C_2H_5O \rightarrow HO_2$ + Products	1.59	7.48
	Total Production	= 21.2 molecules cm^{-3}	
Top 5 Reactions Contributing to HOx Loss			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Loss (%)
1	$HO_2 + NO_2 \rightarrow$ Products	5.21	24.6
2	OH + NC4H10 (n-butane) $\rightarrow$ Products	1.05	4.95
3	$OH + C_3H_8 \rightarrow$ Products	0.949	4.48
4	$OH + CH_3CHO \rightarrow$ Products	0.834	3.93
5	OH + BENZAL (Benzaldehyde) $\rightarrow$ Products	0.609	2.87
	Total Loss	= 21.2 molecules cm^{-3}	

Table S9.2: HOx Production and Loss Budget on Day 4 (SAPRC07 Output)

Top 5 Reactions Contributing to HOx Production			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Production (%)
1	$HNO_4 \rightarrow HO_2$ + Products	8.55	36.0
2	$NO + xHO_2 \rightarrow HO_2$ + Products	8.07	33.9
3	MEO_2 (Methyl peroxy radical) + $NO \rightarrow HO_2$ + Products	1.93	8.11

4	O^1D + $HO_2 \rightarrow OH + OH$	1.78	7.50
5	HCHO + hν → HO_2 + HO_2 + Products	1.69	7.13
	Total Production	= 23.7 molecules cm^{-3}	
Top 5 Reactions Contributing to HOx Loss			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Loss (%)
1	HO_2 + NO_2 → Products	8.81	37.1
2	ALK4 (2-Methylhexane) + OH → Products	3.39	14.3
3	ALK3 (n-Pentane) + OH → Products	2.10	8.85
4	CCHO (Acetaldehyde) + OH → Products	1.47	6.19
5	ALK5 (n-Octane) + OH → Products	1.17	4.94
	Total Loss	= 23.7 molecules cm^{-3}	

Table S9.3: HOx Production and Loss Budget on Day 4 (RACM2 Output)

Top 5 Reactions Contributing to HOx Production			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Production (%)
1	HO_2NO_2 → HO_2 + Products	6.83	30.9
2	HC3P (Peroxy radicals) + NO → HO_2 + Products	2.52	11.4
3	MO2 (Methyl peroxy radical) + NO → HO_2 + Products	2.32	10.5
4	O^1D + $HO_2 \rightarrow OH + OH$	2.13	9.62
5	HCHO → HO_2 + HO_2 + Products	1.99	8.99
	Total Production	= 22.1 molecules cm^{-3}	
Top 5 Reactions Contributing to HOx Loss			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Loss (%)
1	HO_2 + NO_2 → Products	7.11	32.2
2	OH + HC3 → Products	4.16	18.9
3	OH + HC5 → Products	3.02	13.7
4	OH + ACD (Acetaldehyde) → Products	1.52	6.92
5	MACR (Methacrolein) + OH → Products	0.849	3.84
	Total Loss	= 22.1 molecules cm^{-3}	

Table S9.4: HOx Production and Loss Budget on Day 4 (CB6 Output)

Top 5 Reactions Contributing to HOx Production			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Production (%)
1	PNA (Peroxyacetyl nitrate) → HO_2 + Products	14.7	37.8
2	ROR (Alkoxy radicals) → HO_2 + Products	7.62	19.7
3	XO2H (Hydroperoxy alkyl radical) + NO → HO_2 + Products	5.79	14.9
4	O^1D + HO_2 → OH + OH	2.05	5.28
5	FORM (Formaldehyde) → HO_2 + HO_2 + Products	1.54	3.98
	Total Production	= 38.7 molecules cm^{-3}	
Top 5 Reactions Contributing to HOx Loss			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Loss (%)
1	HO_2 + NO_2 → Products	15.3	39.5
2	OH + PAR (Paraffins) → Products	10.7	27.6
3	OH + PRPA (Propionaldehyde) → Products	1.80	4.64
4	OH + ALD2 (Acetaldehyde) → Products	1.40	3.60
5	OH + ALDX (Higher aldehydes)→ Products	1.31	3.39
	Total Loss	= 38.7 molecules cm^{-3}	

Table S10.1: Carbonyl Production and Loss Budget on Day 4 (MCMv331 Output)

Top 5 Reactions Contributing to Formaldehyde (HCHO) Production			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Production (%)
1	CH_3O → HCHO + Products	1.83	55.3
2	CH_3OH + OH → HCHO + Products	0.189	5.70
3	$HOCH_2CH_2O$ → HCHO + HCHO + Products	0.162	4.89
4	C_2H_4 + O_3 → HCHO + Products	0.111	3.35
5	CH_3COCH_2O → HCHO + Products	0.0912	2.76
	Total Production	= 3.31 molecules cm^{-3}	
Reactions Contributing to Formaldehyde (HCHO) Loss			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Loss (%)
1	HCHO + hv → Products	2.35	88.3
2	OH + HCHO → Products	0.309	11.6
3	NO_3 + HCHO → Products	1.30×10^{-3}	0.0491
	Total Loss	= 2.66 molecules cm^{-3}	
Top 5 Reactions Contributing to Acetaldehyde (CH_3CHO) Production			

No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Production (%)
1	$C_2H_5O \rightarrow CH_3CHO$ + Products	1.59	74.9
2	HYPROPO (1-Hydroxypropane-2-yloxy radical) $\rightarrow CH_3CHO$ + Products	0.0689	3.25
3	IPROPOLO (2-Hydroxypropoxy radical) $\rightarrow CH_3CHO$ + Products	0.0610	2.88
4	SC_4H_9O (sec-Butoxy radical) $\rightarrow$ CH_3CHO + Products	0.0576	2.72
5	$C_3H_7CHO + h\nu \rightarrow CH_3CHO$ + Products	0.0556	2.62
	Total Production	= 2.12 molecules cm^{-3}	
Reactions Contributing to Acetaldehyde (CH_3CHO) Loss			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Loss (%)
1	$OH + CH_3CHO \rightarrow$ Products	0.878	83.8
2	$CH_3CHO + h\nu \rightarrow$ Products	0.164	15.8
3	$NO_3 + CH_3CHO \rightarrow$ Products	0.00455	0.435
	Total Loss	= 1.05 molecules cm^{-3}	
Reaction Contributing to Methacrolein (MACR) Production			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Production (%)
1	Emis = MACR	0.511	100
	Total Production	= 0.510 molecules cm^{-3}	
Top 5 Reactions Contributing to Methacrolein (MACR) Loss			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Loss (%)
1	OH + MACR $\rightarrow$ Products	0.122	37.4
2	OH + MACR $\rightarrow$ Products	0.117	35.9
3	O_3 + MACR $\rightarrow$ Products	0.0258	7.91
4	OH + MACR $\rightarrow$ Products	0.0207	6.36
5	MACR + $h\nu \rightarrow$ Products	0.0178	5.48
	Total Loss	= 0.330 molecules cm^{-3}	
Top 5 Reactions Contributing to Benzaldehyde (BENZAL) Production			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Production (%)
1	Emis $\rightarrow$ BENZAL	1.69	99.3
2	$C_6H_5CH_2O \rightarrow$ BENZAL + Products	0.0117	0.688
3	$C_6H_5CH_2OOH + OH \rightarrow$ BENZAL + Products	3.07×10^{-4}	0.0181
4	$C_6H_5CH_2NO_3 + OH \rightarrow$ BENZAL + Products	2.81×10^{-4}	0.0165
5	$C_6H_5CH_2O_2 + RO_2$ = BENZAL	4.53×10^{-5}	0.00267
	Total Production	= 1.70 molecules cm^{-3}	
Reactions Contributing to Benzaldehyde (BENZAL) Loss			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Loss (%)
1	OH + BENZAL $\rightarrow$ Products	0.609	74.3
2	BENZAL + $h\nu \rightarrow$ Products	0.203	24.9
3	NO_3 + BENZAL $\rightarrow$ Products	7.32×10^{-3}	0.893
	Total Loss	= 0.820 molecules cm^{-3}	

Top 5 Reactions Contributing to Methyl Ethyl Ketone (MEK) Production			
No.	Reaction	Integrated Reaction Rate (molecules cm⁻³)	Percent of Production (%)
1	SC_4H_9O → MEK + Products	0.876	84.4
2	M_3PECO (1-Methyl-1-ethylpropoxyradical) → MEK + Products	0.123	11.9
3	OH + SC_4H_9OOH (sec-butyl hydroperoxide) → MEK + Products	0.0282	2.72
4	M_2BKBO → MEK + Products	0.00358	0.345
5	OH + $SC_4H_9NO_3$ (sec-Butyl Nitrate)→ MEK + Products	0.00313	0.301
	Total Production	= 1.04 molecules cm^{-3}	
Reactions Contributing to Methyl Ethyl Ketone (MEK) Loss			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Loss (%)
1	MEK + hν → Products	0.111	72.0
2	MEK + OH → Products	0.0199	12.9
3	MEK + OH → Products	0.0197	12.9
4	MEK + OH → Products	0.00340	2.21
	Total Production	= 0.150 molecules cm^{-3}	

Table S10.2: Carbonyl Production and Loss Budget on Day 4 (SAPRC07 Output)

Top 5 Reactions Contributing to Formaldehyde (HCHO) Production			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Production (%)
1	MEO_2 (Methyl peroxy radical) + NO → HCHO + Products	1.91	59.2
2	NO + xHCHO → HCHO + Products	0.738	22.7
3	MEOH + OH → HCHO + Products	0.167	5.15
4	$MACO_3$ (Methacryloyl peroxy radical) + NO → HCHO + Products	0.114	3.51
5	ETHE (Ethene) + O_3 → HCHO + Products	0.114	3.51
	Total Production	= 3.25 molecules cm^{-3}	
Reactions Contributing to Formaldehyde (HCHO) Loss			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Loss (%)
1	HCHO + hν → Products	2.35	89.5
2	OH + HCHO → Products	0.275	10.5
3	NO_3 + HCHO → Products	0.00144	0.0550
	Total Loss	= 2.62 molecules cm^{-3}	
Top 5 Reactions Contributing to Acetaldehyde (CCHO) Production			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Production (%)
1	NO + xCCHO = CCHO + Products	3.71	98.3
2	NO_3 + xCCHO = CCHO + Products	0.0183	0.485
3	RNO_3 + hν = 0.21 CCHO + Products	0.0157	0.415
4	OLE1 (Terminal alkene) + O_3 = 0.15 CCHO + Products	0.0145	0.385

5	$MECO_3$ (2-butanoyl peroxy radical) + xCCHO = CCHO + Products	0.00782	0.207
	Total Production	= 3.77 molecules cm^{-3}	
Reactions Contributing to Acetaldehyde (CCHO) Loss			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Loss (%)
1	OH + CCHO → Products	1.47	81.6
2	CCHO + hν → Products	0.308	17.1
3	NO_3 + CCHO → Products	0.0247	1.37
	Total Loss	= 1.80 molecules cm^{-3}	
Top 5 Reactions Contributing to Methacrolein (MACR) Production			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Production (%)
1	Emis → MACR	1.02	99.8
2	NO + xMACR → MACR + Products	0.00215	0.210
3	AFG3 (Aromatic dicarbonyl fragment) + O_3 → MACR + Products	0.000187	0.0183
4	NO_3 + xMACR → MACR + Products	1.20×10^{-5}	0.00117
5	$MECO_3$ + xMACR → MACR + Products	4.45×10^{-6}	0.000434
	Total Production	= 1.03 molecules cm^{-3}	
Top 5 Reactions Contributing to Methacrolein (MACR) Loss			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Loss (%)
1	MACR + OH → Products	0.513	76.7
2	MACR + hν → Products	0.0809	12.1
3	MACR + O_3 → Products	0.0678	10.1
4	MACR + NO_3 → Products	0.00551	0.823
5	MACR + O^3P → Products	0.00158	0.236
	Total Loss	= 0.670 molecules cm^{-3}	
Top 5 Reactions Contributing to Benzaldehyde (BALD) Production			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Production (%)
1	Emis → BALD	1.50	98.8
2	NO + xBALD → BALD + Products	0.0183	1.20
3	NO_3 + xBALD → BALD + Products	0.000100	0.00660
4	MECO3 + xBALD → BALD + Products	3.84×10^{-5}	0.00252
5	RCO_3 + xBALD → BALD + Products	1.38×10^{-5}	0.000905
	Total Production	= 1.52 molecules cm^{-3}	
Reactions Contributing to Benzaldehyde (BALD) Loss			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Loss (%)
1	OH + BALD → Products	0.515	97.0
2	NO_3 + BALD → Products	0.0119	2.25
3	BALD + hν → Products	0.00379	0.714
	Total Loss	= 0.530 molecules cm^{-3}	
Top 5 Reactions Contributing to Methyl Ethyl Ketone (MEK) Production			

No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Production (%)
1	NO + xMEK → MEK + Products	1.43	98.1
2	RNO_3 + hv → 0.12 MEK + Products	0.00908	0.623
3	NO_3 + xMEK → MEK + Products	0.00772	0.530
4	$MECO_3$ + xMEK → MEK + Products	0.00294	0.202
5	RNO_3 + OH → 0.01 MEK + Products	0.00287	0.197
	Total Production	= 1.46 molecules cm^{-3}	
Reactions Contributing to Methyl Ethyl Ketone (MEK) Loss			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Loss (%)
1	MEK + OH → Products	0.0507	63.5
2	MEK + hν → Products	0.0291	36.5
	Total Production	= 0.0800 molecules cm^{-3}	

Table S10.3: Carbonyl Production and Loss Budget on Day 4 (RACM2 Output)

Top 5 Reactions Contributing to Formaldehyde (HCHO) Production			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Production (%)
1	MO2 (Methyl peroxy radical) + NO → HCHO + Products	2.32	59.8
2	ETEP (Peroxy radicals formed from ethene) + NO → 1.6 HCHO + Products	0.354	9.10
3	HKET → HCHO + Products	0.328	8.46
4	MCP + NO → 0.5 HCHO + Products	0.173	4.47
5	OH + MOH → HCHO + Products	0.165	4.25
	Total Production	= 3.88 molecules cm^{-3}	
Reactions Contributing to Formaldehyde (HCHO) Loss			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Loss (%)
1	HCHO → Products	2.75	89.8
2	OH + HCHO → Products	0.312	10.2
3	NO_3 + HCHO → Products	0.00160	0.0521
	Total Loss	= 3.06 molecules cm^{-3}	
Top 5 Reactions Contributing to Acetaldehyde (ACD) Production			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Production (%)
1	ETHP + NO → ACD + Products	1.93	48.0
2	HC3P (Peroxy radicals) + NO → ACD + Products	1.92	47.9
3	HC5P (Peroxy radicals) + NO → ACD + Products	0.12	3.00
4	OH + EOH → ACD + Products	0.0176	0.438
5	OH + ROH → 0.18 ACD + Products	0.0110	0.273
	Total Production	= 4.02 molecules cm^{-3}	
Reactions Contributing to Acetaldehyde (ACD) Loss			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Loss (%)
1	OH + ACD → Products	1.53	81.5
2	ACD → Products	0.325	17.3

3	NO_3 + ACD → Products	0.0221	1.18
	Total Loss	= 1.88 molecules cm^{-3}	
Reaction Contributing to Methacrolein (MACR) Production			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Production (%)
1	Emis → MACR	1.78	100
	Total Production	= 1.78 molecules cm^{-3}	
Top 5 Reactions Contributing to Methacrolein (MACR) Loss			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Loss (%)
1	MACR + OH → Products	0.513	76.721
2	MACR → Products	0.0809	12.1
3	MACR + O_3 → Products	0.0678	10.1
4	MACR + NO_3 → Products	0.00551	0.823
	Total Loss	= 1.10 molecules cm^{-3}	
Top 5 Reactions Contributing to Benzaldehyde (BALD) Production			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Production (%)
1	EPX (Epoxide) + O_3 → BALD + Products	0.107	72.1
2	PER1 (Peroxy intermediate formed from toluene) + NO → 0.5 BALD + Products	0.0199	13.4
3	TLP1 (Peroxy radicals) + NO → BALD + Products	0.0103	6.90
4	XYL1 (Peroxy radicals) + NO → BALD + Products	0.00945	6.36
5	OLT (Terminal alkenes) + O_3 → BALD + Products	0.00169	1.14
	Total Production	= 0.150 molecules cm^{-3}	
Reactions Contributing to Benzaldehyde (BALD) Loss			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Loss (%)
1	OH + BALD → Products	0.0810	89.9
2	BALD → HO_2 + Products	0.00913	10.1
	Total Loss	= 0.0900 molecules cm^{-3}	
Top 5 Reactions Contributing to Methyl Ethyl Ketone (MEK) Production			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Production (%)
1	HC3P + NO → MEK + Products	0.160	60.5
2	HC5P + NO → MEK + Products	0.0883	33.3
3	OLTP + NO → MEK + Products	0.00901	3.40
4	OLT + O_3 → MEK + Products	0.00507	1.91
5	DCB2 (Unsaturated dicarbonyl) + OH → MEK + Products	0.00106	0.399
	Total Production	= 0.270 molecules cm^{-3}	
Reactions Contributing to Methyl Ethyl Ketone (MEK) Loss			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Loss (%)
1	MEK → Products	0.0285	72.6

2	MEK + OH → Products	0.0108	27.4
	Total Production	= 0.040 molecules cm^{-3}	

Table S10.4: Carbonyl Production and Loss Budget on Day 4 (CB6 Output)

Top 5 Reactions Contributing to Formaldehyde (FORM) Production			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Production (%)
1	MEO2 (Methyl peroxy radical) + NO → FORM + Products	1.54	36.0
2	HCO3 (Formyl peroxy radical) → FORM + Products	1.12	26.2
3	OH + ETH → 1.56 FORM + Products	0.500	11.7
4	OH + OLE → 0.78 FORM + Products	0.335	7.83
5	MEOH (Methanol) + OH → FORM + Products	0.263	6.14
	Total Production	= 4.28 molecules cm^{-3}	
Reactions Contributing to Formaldehyde (FORM) Loss			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Loss (%)
1	FORM → Products	2.14	58.39
2	FORM + HO_2 → Products	1.13	30.76
3	FORM + OH → Products	0.393	10.74
4	FORM + NO_3 → Products	0.00401	0.110
5	FORM + O^3P → Products	4.09×10^{-5}	0.00112
	Total Loss	= 3.66 molecules cm^{-3}	
Top 5 Reactions Contributing to Acetaldehyde (ALD2) Production			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Production (%)
1	OH + ETHA → 0.991 ALD2 + Products	0.668	23.3
2	CXO3 (Acyl peroxy radical) + NO → ALD2 + Products	0.536	18.7
3	KET → 0.58 ALD2 + Products	0.479	16.7
4	ROR → 0.74 ALD2 + Products	0.385	13.4
5	ALDX → ALD2 + Products	0.260	9.07
	Total Production	= 2.86 molecules cm^{-3}	
Reactions Contributing to Acetaldehyde (ALD2) Loss			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Loss (%)
1	ALD2 + OH → Products	1.39	87.2
2	ALD2 → Products	0.188	11.7
3	ALD2 + NO_3 → Products	0.0162	1.01
4	ALD2 + O^3P → Products	0.000264	0.0165
	Total Loss	= 1.60 molecules cm^{-3}	
Top 5 Reactions Contributing to the Production of Aldehydes with Three or More Carbon Atoms (ALDX)			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Production (%)
1	OH + PAR → 0.11 ALDX + Products	1.18	48.1

2	OH + PRPA (Propionaldehyde) → 0.26 ALDX + Products	0.467	19.1
3	KET → 0.58 ALD2 + Products	0.281	11.5
4	OH + OLE → 0.488 ALDX + Products	0.210	8.57
5	ROR (Alkoxy radical) → 0.37 ALDX + Products	0.192	7.87
	Total Production	= 2.44 molecules cm^{-3}	
Reactions Contributing to the Loss of Aldehydes with Three or More Carbon Atoms (ALDX)			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Loss (%)
1	ALDX + OH → Products	1.31	80.3
2	ALDX → Products	0.260	15.9
3	ALDX + NO_3 → Products	0.0610	3.74
4	ALDX + O^3P → Products	0.000324	0.0198
	Total Loss	= 1.63 molecules cm^{-3}	
Top 5 Reactions Contributing to Ketone Species (KET) Production			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Production (%)
1	ROR → KET + Products	7.62	98.7
2	ROR → 0.2 KET + Products	0.104	1.35
	Total Production	= 7.72 molecules cm^{-3}	
Reactions Contributing to Ketone Species (KET) Loss			
No.	Reaction	Integrated Reaction Rate (molecules cm^{-3})	Percent of Loss (%)
1	KET → Products	0.827	100
	Total Loss	= 0.827 molecules cm^{-3}	