Supplementary Information

An Updated Modeling Framework to Simulate Los Angeles Air Quality. Part 1: Model Development, Evaluation, and Source Apportionment.

Elyse A. Pennington, et al.

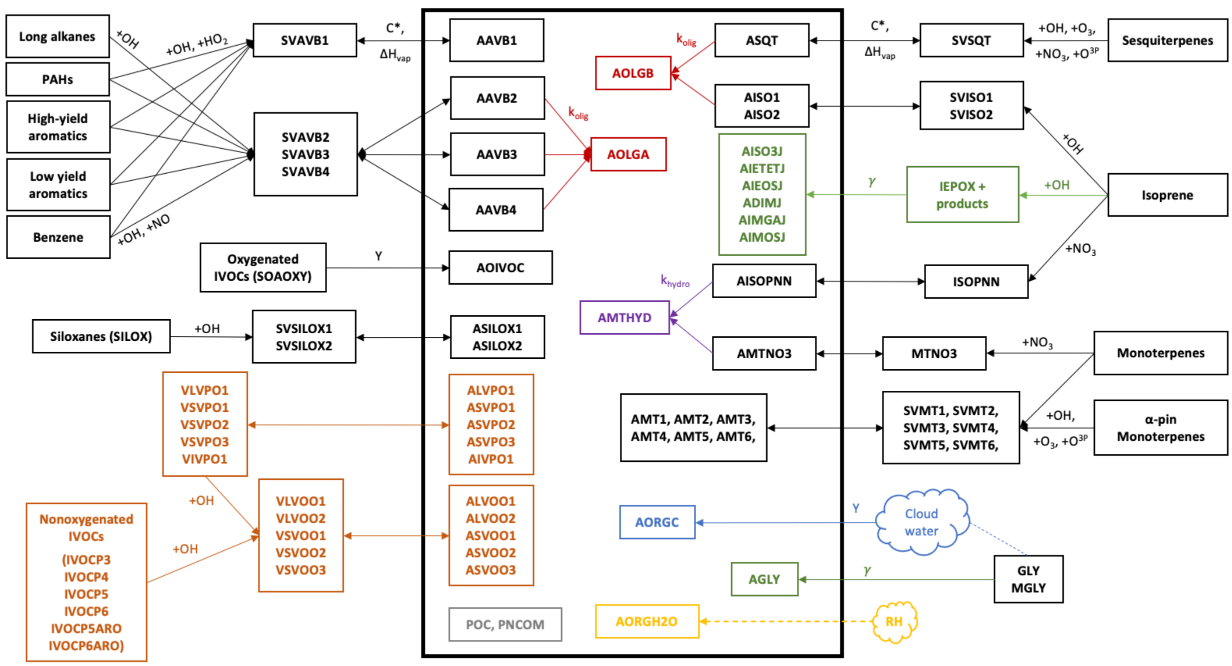

Figure S1: Schematic of OA chemical mechanism used in these simulations. It includes AERO7 and additional VCP (Pennington et al., 2021) and mobile IVOC (Lu et al., 2020) emissions and chemistry.

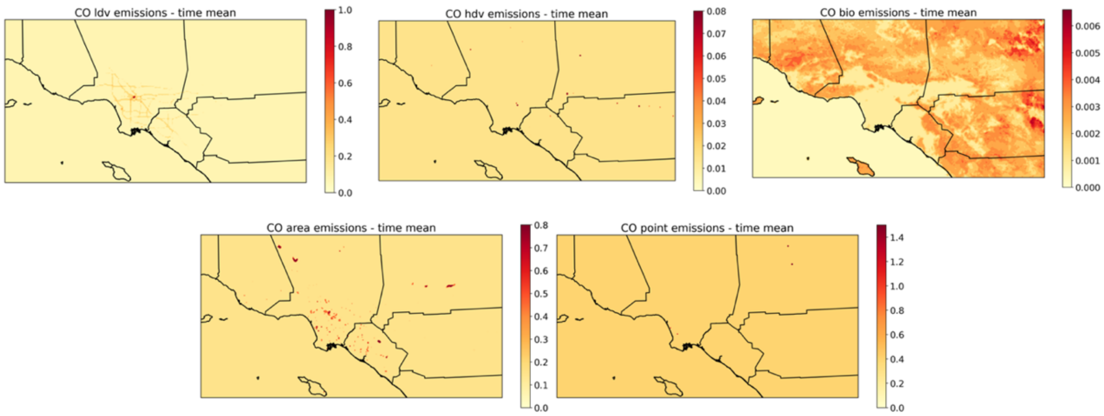

Figure S2: Time-averaged (April 1–30, 2020) emission rate (tons/day) of CO from a) light duty on-road vehicles, b) heavy duty on-road vehicles, c) biogenic, d) area, and e) point sources.

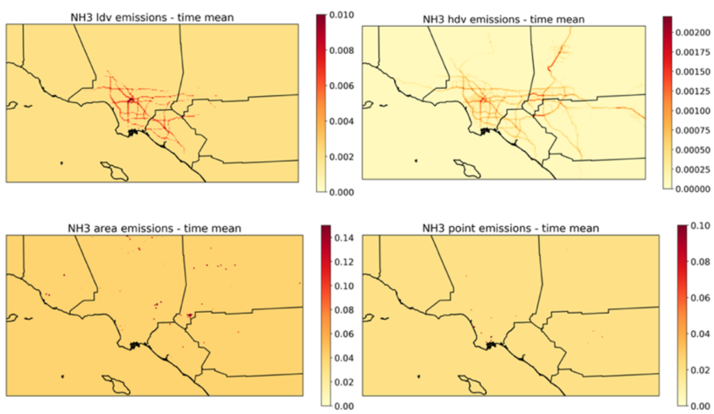

Figure S3: Time-averaged (April 1–30, 2020) emission rate (tons/day) of NH_3 from a) light duty on-road vehicles, b) heavy duty on-road vehicles, c) area, and d) point sources.

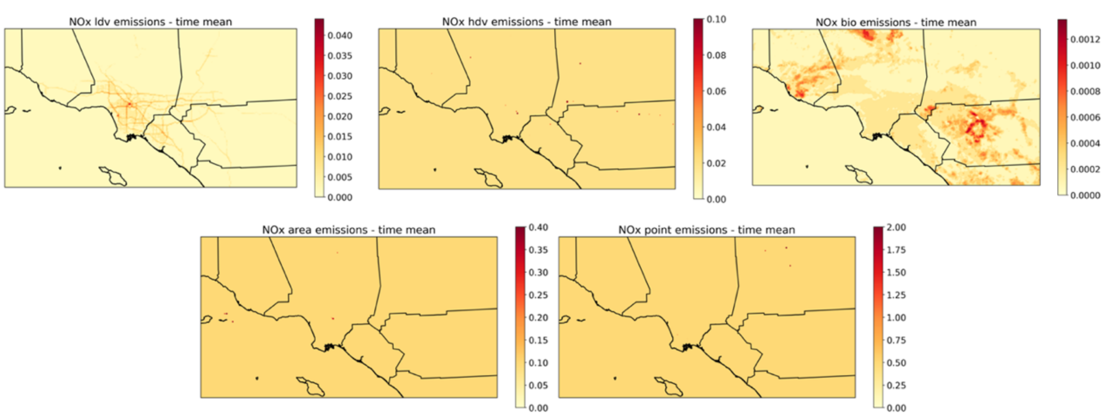

Figure S4: Time-averaged (April 1–30, 2020) emission rate (tons/day) of NO_x from a) light duty on-road vehicles, b) heavy duty on-road vehicles, c) biogenic, d) area, and e) point sources.

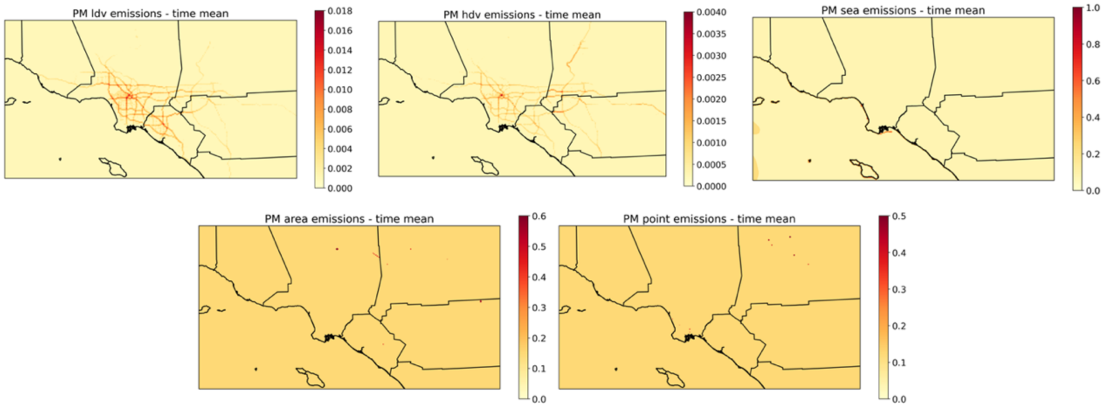

Figure S5: Time-averaged (April 1–30, 2020) emission rate (tons/day) of PM from a) light duty on-road vehicles, b) heavy duty on-road vehicles, c) sea spray, d) area, and e) point sources.

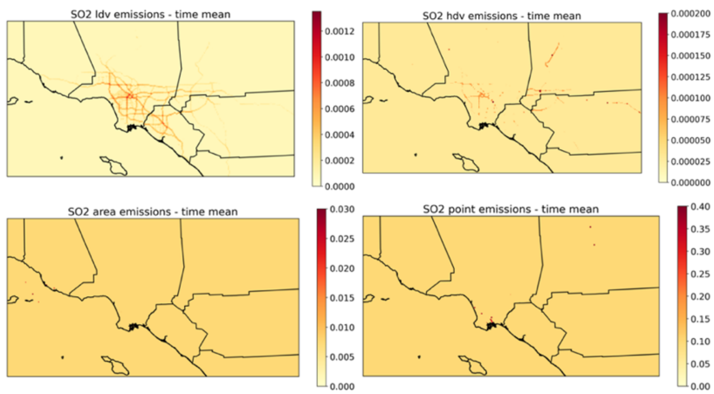

Figure S6: Time-averaged (April 1–30, 2020) emission rate (tons/day) of SO_2 from a) light duty on-road vehicles, b) heavy duty on-road vehicles, c) area, and d) point sources.

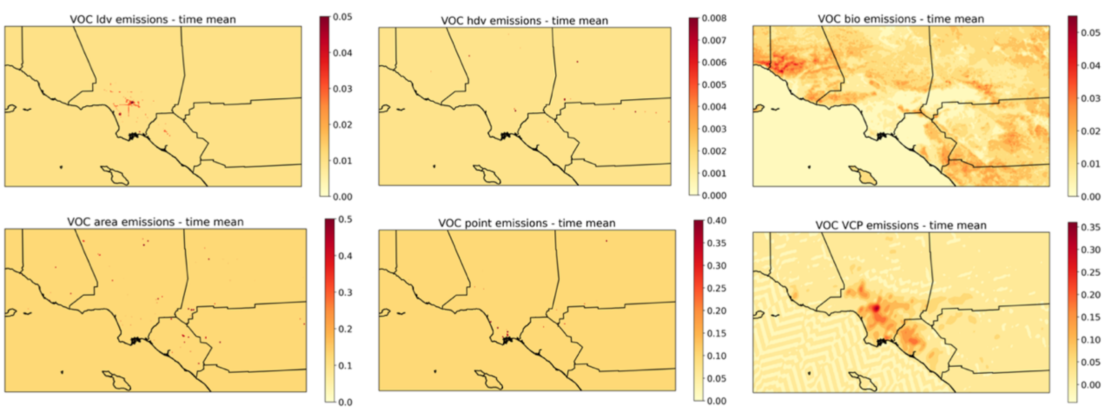

Figure S7: Time-averaged (April 1–30, 2020) emission rate (tons/day) of VOCs from a) light duty on-road vehicles, b) heavy duty on-road vehicles, c) biogenic, d) area, e) point, and f) VCP sources.

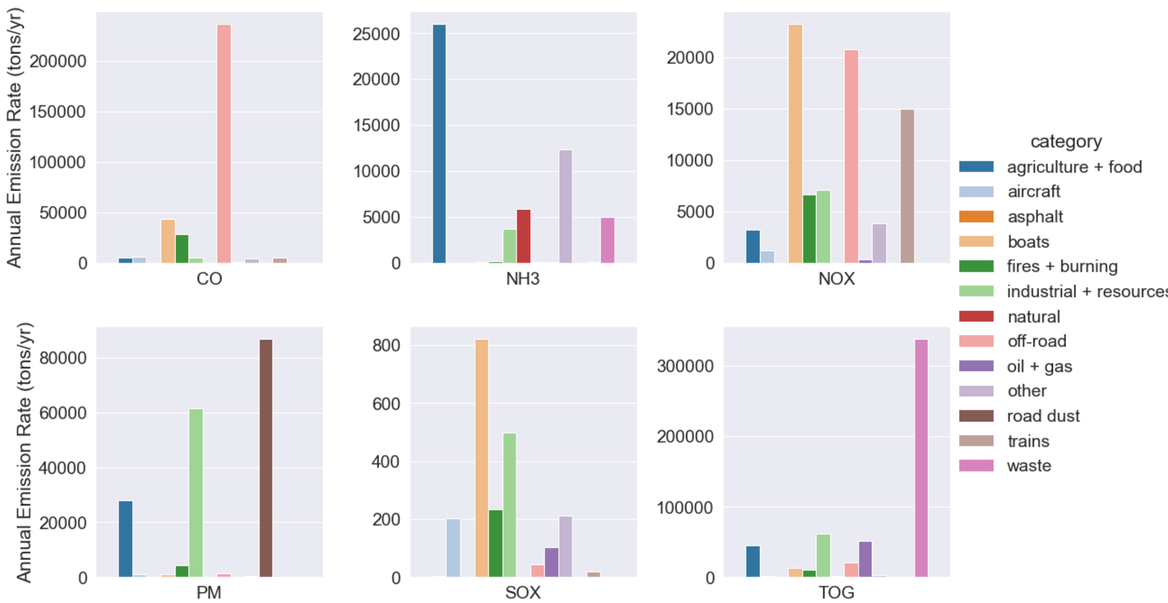

Figure S8: Annual emission rates of pollutants in CARB area source emissions inventory.

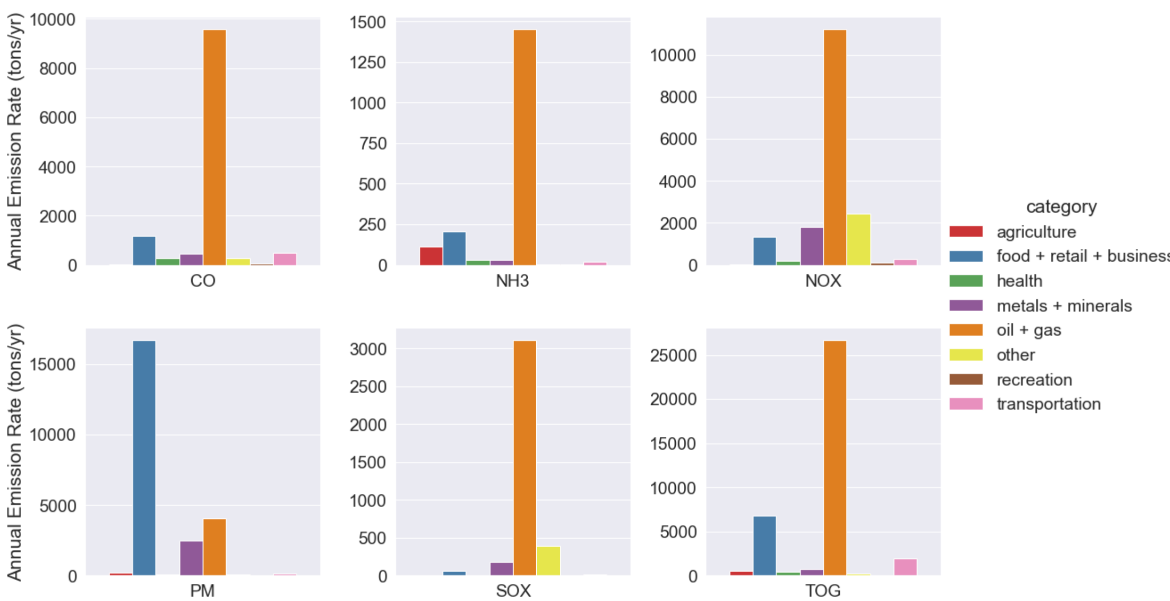

Figure S9: Annual emission rates of pollutants in CARB point source emissions inventory.

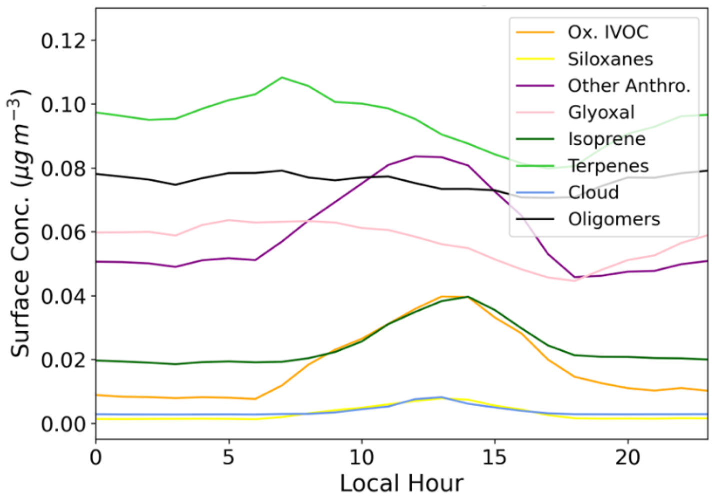

Figure S10: Same as Figure 8C with POA, alkane-like IVOCs, and organic nitrates removed.

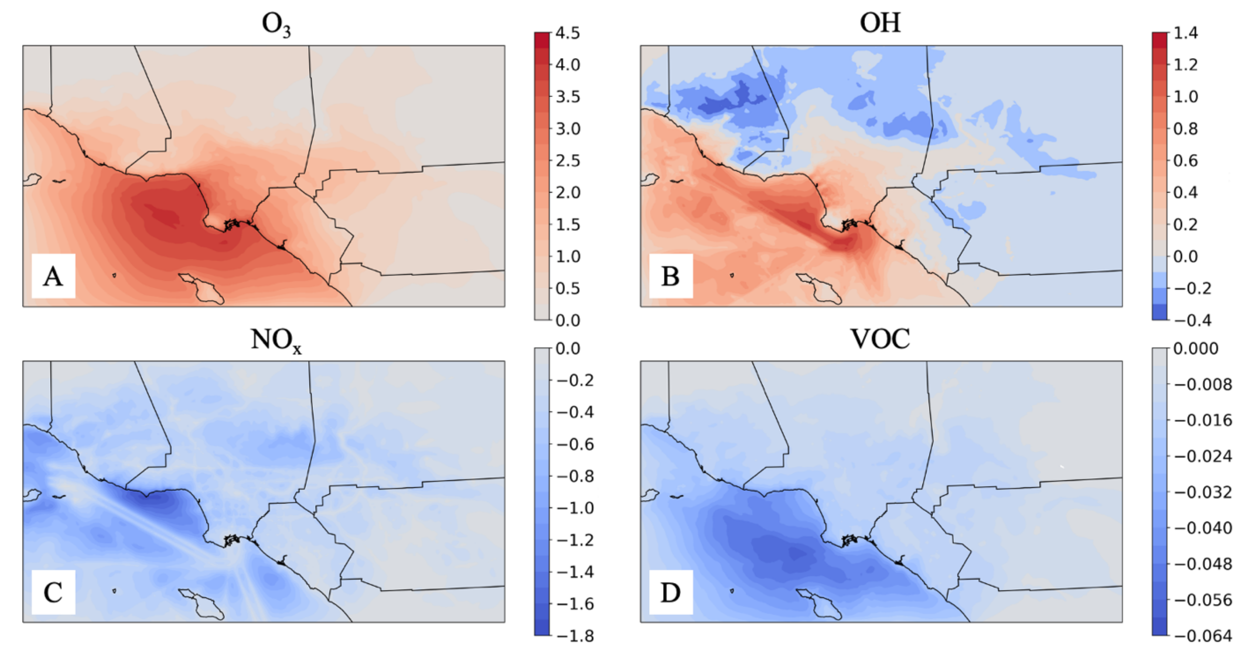

Figure S11: Percent change in average predicted A) O_3, B) OH, C) NO_x, D) VOC concentrations caused by removing sea spray emissions.

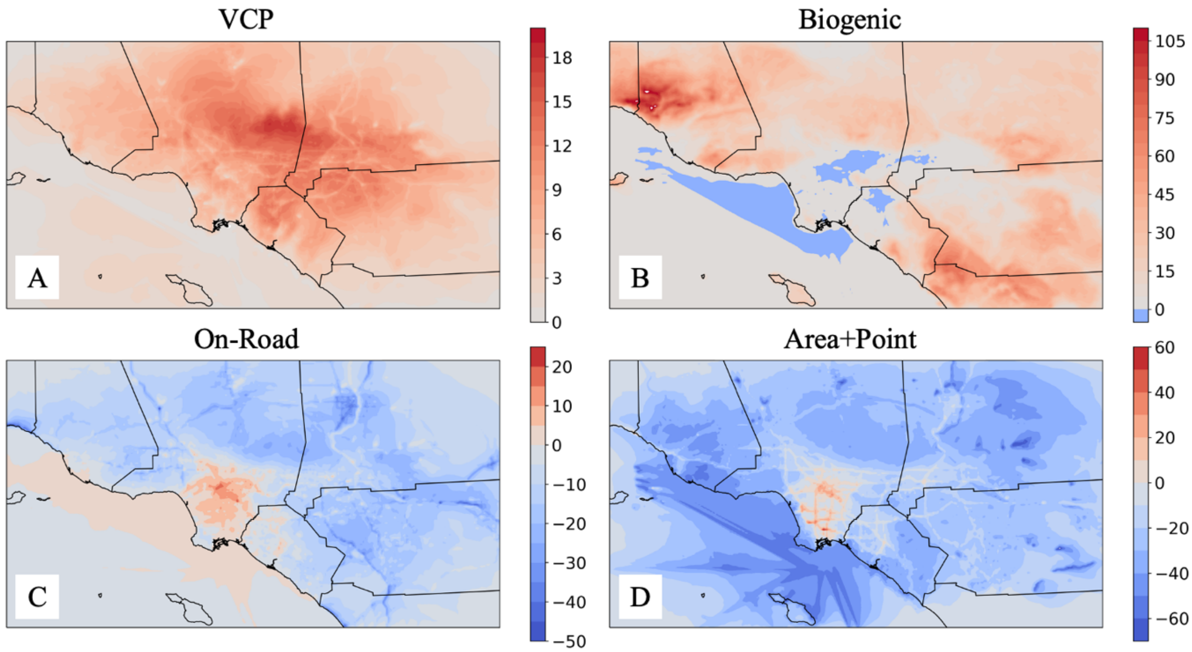

Figure S12: Percent change in average predicted OH concentration caused by removing each emission source: A) VCP emissions B) biogenic emissions C) on-road vehicle emissions D) area+point emissions.

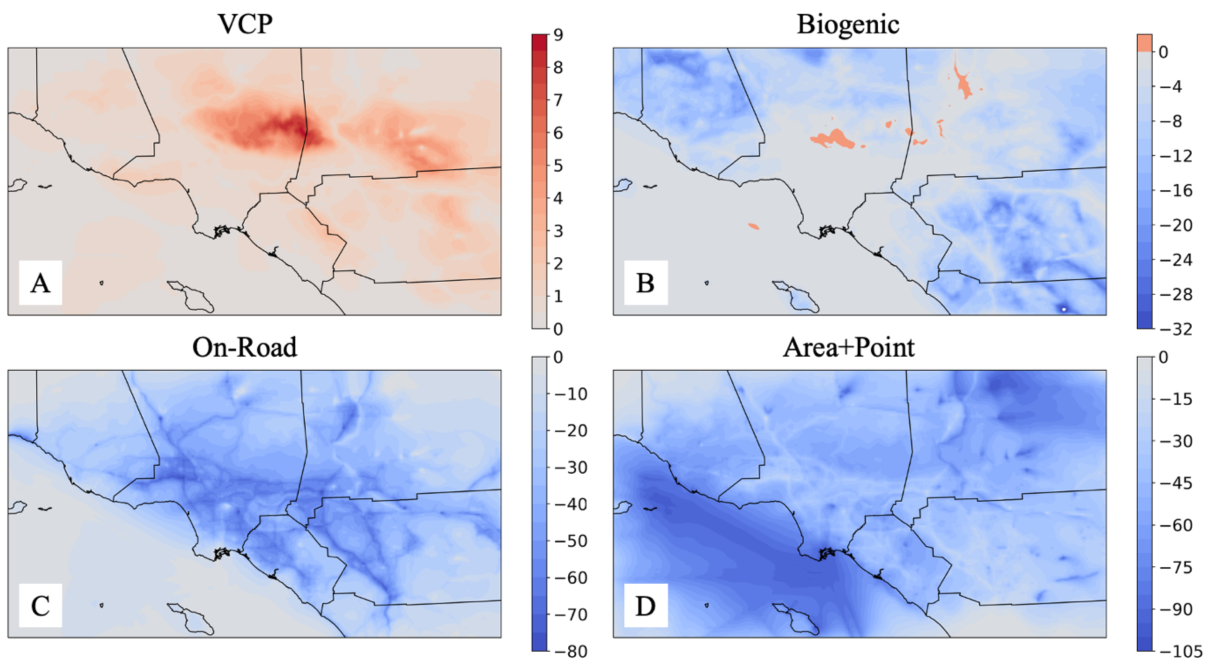

Figure S13: Percent change in average predicted NO_x concentration caused by removing each emission source: A) VCP emissions B) biogenic emissions C) on-road vehicle emissions D) area+point emissions.

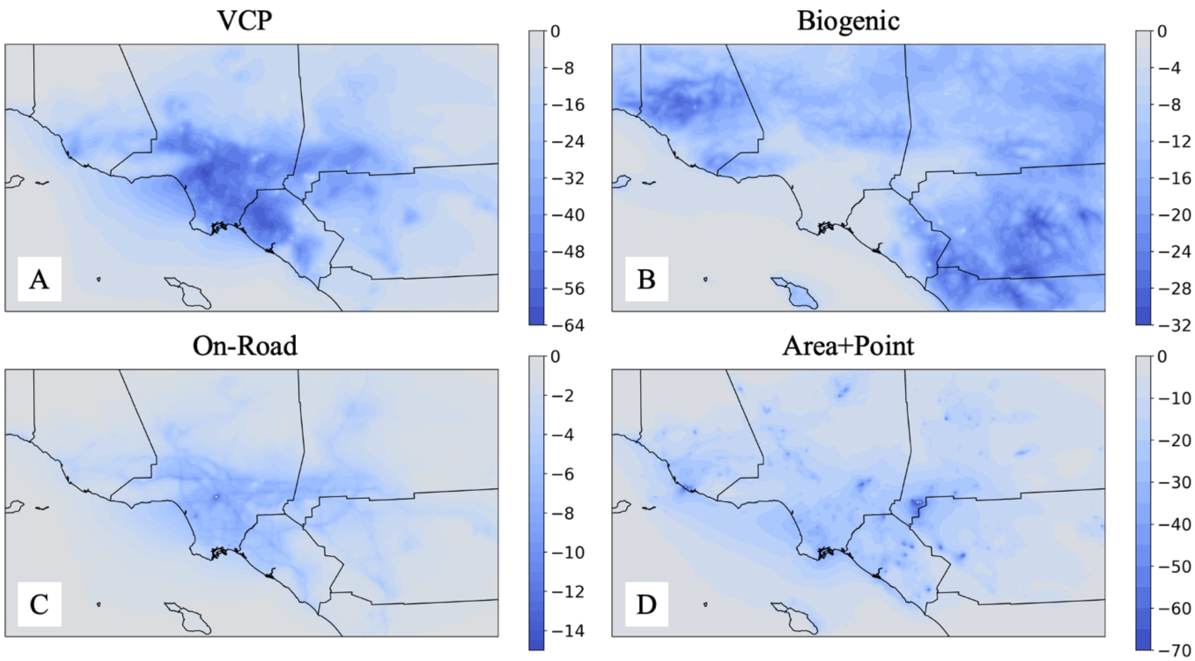

Figure S14: Percent change in average predicted VOC concentration caused by removing each emission source: A) VCP emissions B) biogenic emissions C) on-road vehicle emissions D) area+point emissions.

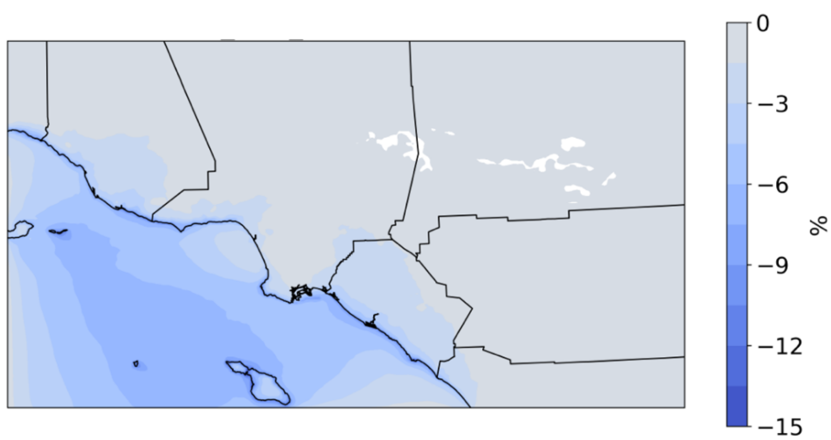

Figure S15: Percent change in average predicted $PM_{2.5}$ concentration caused by removing sea spray emissions.

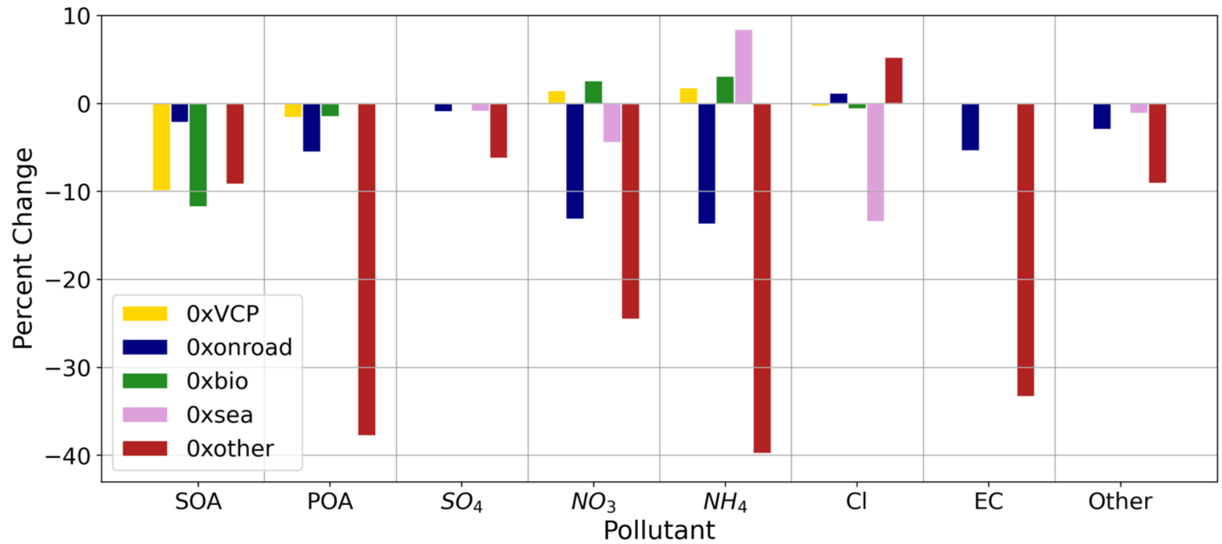

Figure S16: Percent change of $PM_{2.5}$ components averaged over the LA domain when each emission source is removed.

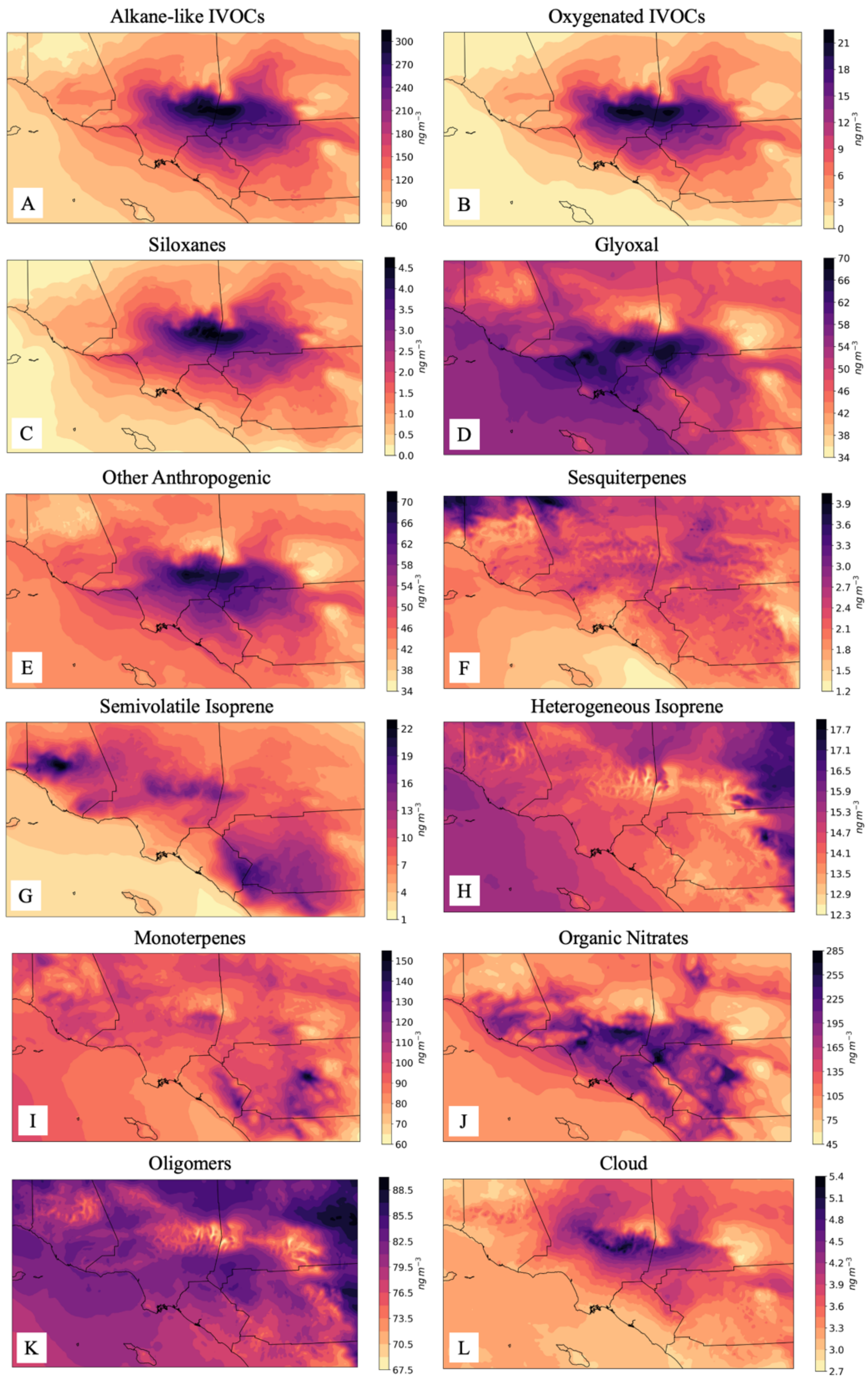

Figure S17: Time-averaged (April 1–30, 2020) CMAQ predicted concentrations (ng m^{-3}) of SOA components derived from: A) alkane-like IVOCs, B) oxygenated IVOCs, C) siloxanes, D) glyoxal, E) other anthropogenic sources, F) sesquiterpenes, G) semivolatile isoprene, H) heterogeneous isoprene, I) monterpenes, J) organic nitrates, K) oligomers, and L) clouds. The star is located on Pasadena.

Table S1: Statistical analysis of daily-averaged WRF predictions compared to EPA AQS monitoring site data.

	Temperature	Relative Humidity	Wind Speed	Wind Direction
Observed Mean	17.19 °C	65.7%	1.43 m s^{-1}	233.1°
Modeled Mean	17.84 °C	51.7%	2.12 m s^{-1}	194.2°
MB	0.65 °C	-14.0%	0.68 m s^{-1}	-38.8°
NMB	3.80%	-21.3%	47.7%	-16.7%
RMSE	1.14 °C	16.5%	0.81 m s^{-1}	57.5°
r^2	0.97	0.81	0.08	0.26

Table S2: Statistical analysis of daily-averaged CMAQ predictions in the LA domain compared to EPA AQS monitoring site data.

	O_3	CO	NO_x	SO_2	$PM_{2.5}$
Observed Mean	33.76 ppb	228.8 ppb	12.4 ppb	195.3 ppt	9.11 μg m^{-3}
Modeled Mean	37.19 ppb	139.1 ppb	4.72 ppb	91.9 ppt	6.92 μg m^{-3}
MB	3.43 ppb	-89.8 ppb	-7.65 ppb	-103.4 ppt	-2.19 μg m^{-3}
NMB	10.2%	-39.2%	-61.9%	-52.9%	-24.0 %
RMSE	6.21 ppb	112.8 ppb	11.3 ppb	120.7 ppt	3.74 μg m^{-3}
r^2	0.30	0.36	0.15	0.47	0.82

Table S3: Statistical analysis of daily-averaged CMAQ predictions in Pasadena compared to Caltech AMS data.

	Observed Mean	Modeled Mean	MB	NMB	RMSE	r^2
PM_1	6.395 μg m^{-3}	3.258 μg m^{-3}	-3.14 μg m^{-3}	-49.1%	-	-
PM_1 SO_4	0.953 μg m^{-3}	0.754 μg m^{-3}	-0.199 μg m^{-3}	-20.8%	0.419 μg m^{-3}	0.79
PM_1 NO_3	0.696 μg m^{-3}	0.600 μg m^{-3}	-0.096 μg m^{-3}	-13.8%	0.735 μg m^{-3}	0.045
PM_1 NH_4	0.475 μg m^{-3}	0.125 μg m^{-3}	-0.350 μg m^{-3}	-73.5%	0.519 μg m^{-3}	0.0
PM_1 Cl	0.060 μg m^{-3}	0.013 μg m^{-3}	-0.047 μg m^{-3}	-77.8%	0.063 μg m^{-3}	0.19
PM_1 OM	4.211 μg m^{-3}	1.556 μg m^{-3}	-2.66 μg m^{-3}	-63.0%	-	-
PM_1 POM	0.668 μg m^{-3}	0.767 μg m^{-3}	-0.099 μg m^{-3}	-14.8%	-	-
PM_1 SOM	2.502 μg m^{-3}	0.789 μg m^{-3}	-1.713 μg m^{-3}	-68.5%	-	-

Table S4: Statistical analysis of daily-averaged CMAQ predictions in Pasadena compared to CITAQS data.

	Observed Mean	Modeled Mean	MB	NMB	RMSE	r^2
O_3	35.6 ppb	35.9 ppb	0.33 ppb	0.94%	4.49 ppb	0.56
CO	232 ppb	169 ppb	-63.0 ppb	-27.2%	72.0 ppb	0.72
SO_2	0.077 ppb	0.158 ppb	0.081 ppb	105%	0.112 ppb	0.39
NO	0.762 ppb	0.579 ppb	-0.183 ppb	-24.0%	0.524 ppb	0.26
NO_2	8.18 ppb	4.99 ppb	-3.19 ppb	-39.0%	3.84 ppb	0.45
NO_x	8.20 ppb	5.57 ppb	-2.63 ppb	-32.1%	3.80 ppb	0.21
$PM_{2.5}$	9.10 μg m^{-3}	7.91 μg m^{-3}	-1.20 μg m^{-3}	-13.1%	3.28 μg m^{-3}	0.71
PM_{10}	19.85 μg m^{-3}	23.06 μg m^{-3}	3.20 μg m^{-3}	16.1%	5.65 μg m^{-3}	0.80
Temperature	18.6 °C	18.4 °C	-0.25 °C	-1.34%	1.14 °C	0.95

Table S6: Mass concentration change (ng m^{-3}) of SOA components in Pasadena averaged April 1–30, 2020 when each emission source is removed.

ng m^{-3}	VCP	On-Road	Biogenic	Sea Spray	Area+Point
Alkane-like IVOCs	-109.74	-6.91	-1.39	0.21	-65.45
Oxygenated IVOCs	-19.03	-0.40	-0.21	0.04	-0.80
Siloxanes	-3.21	-0.04	-0.08	4.6×10^{-3}	-0.50
Glyoxal	-3.31	-3.75	-5.05	-0.22	-9.50
Other anthropogenic	-13.70	-2.90	-2.67	0.29	-8.98
Isoprene	-1.09	-0.33	-8.92	6.8×10^{-3}	-2.25
Monoterpenes	-9.44	1.44	-18.94	-0.06	-6.58
Sesquiterpenes	-0.38	-0.17	-0.24	3.6×10^{-4}	-0.98
Organic nitrates	-60.26	-17.24	-107.62	0.56	-61.57
Oligomers	-1.75	-0.57	-2.26	5.0×10^{-4}	-1.72
Cloud-processed	-0.35	-0.16	-0.18	1.8×10^{-3}	-0.60

References

Lu, Q., Murphy, B. N., Qin, M., Adams, P. J., Zhao, Y., Pye, H. O. T., Efstathiou, C., Allen, C., & Robinson, A. L. (2020). Simulation of organic aerosol formation during the CalNex study: Updated mobile emissions and secondary organic aerosol parameterization for intermediate-volatility organic compounds. *Atmospheric Chemistry and Physics*, *20*(7), 4313–4332. https://doi.org/10.5194/acp-20-4313-2020

Pennington, E. A., Seltzer, K. M., Murphy, B. N., Qin, M., Seinfeld, J. H., & Pye, H. O. T. (2021). Modeling secondary organic aerosol formation from volatile chemical products. *Atmospheric Chemistry and Physics*, *21*(24), 18247–18261. https://doi.org/10.5194/acp-21-18247-2021