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Understanding sources of organic aerosol during CalNex-2010 using the CMAQ-VBS

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Table S1: Comparison of CMAQ-AE6 and CMAQ-VBS POA treatments.

Model	Functionalization	Volatility
CMAQ-AE6	Non-carbon organic matter added via 2nd order reaction between reduced primary organic carbon and OH	Nonvolatile
CMAQ-VBS	Gas-phase semivolatile aged by OH	Semivolatile

Table S2: Comparisons of CMAQ-AE6 and CMAQ-VBS SOA treatments.

CMAQ-AE6 (Carlton et al., 2010)			
SOA Precursor	Precursor Oxidant	Aging	NO_x Dependent Yields?
Monoterpene	O, OH O_3, NO_3	Oligomerization (particle-phase aging)	No
Sesquiterpene	OH, O_3, NO_3	”	No
Isoprene	OH	”	No
Xylene	OH	”	Yes
Benzene	OH	”	Yes
Toluene	OH	”	Yes
CMAQ-VBS (Koo et al., 2014)			
SOA Precursor	Precursor Oxidant	Aging	NO_x Dependent Yields?
Monoterpene	OH, O_3, NO_3	None	Yes
Sesquiterpene	OH, O_3, NO_3	None	No
Isoprene	O3, NO3, OH	None	Yes
Xylene	OH	Gas-phase semivolatile aged by OH	Yes
Benzene	OH	”	Yes
Toluene	OH	”	Yes

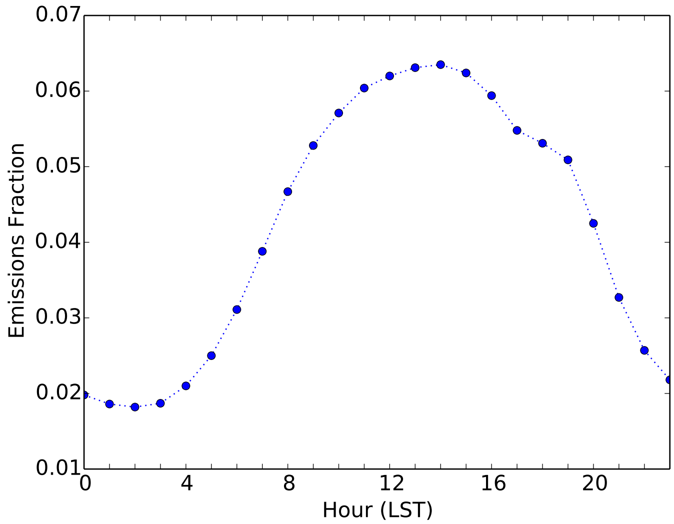


Figure S1: SMOKE diurnal profile 26 applied to majority of meat cooking POA emissions in domain.

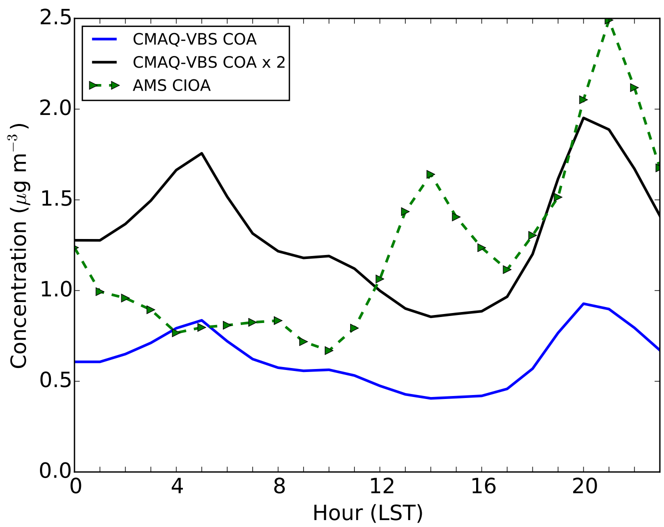


Figure S2: Diurnal profile of CMAQ-VBS CIOA, CMAQ-VBS CIOA emissions increased by 2, and AMS-measured CIOA at Pasadena.

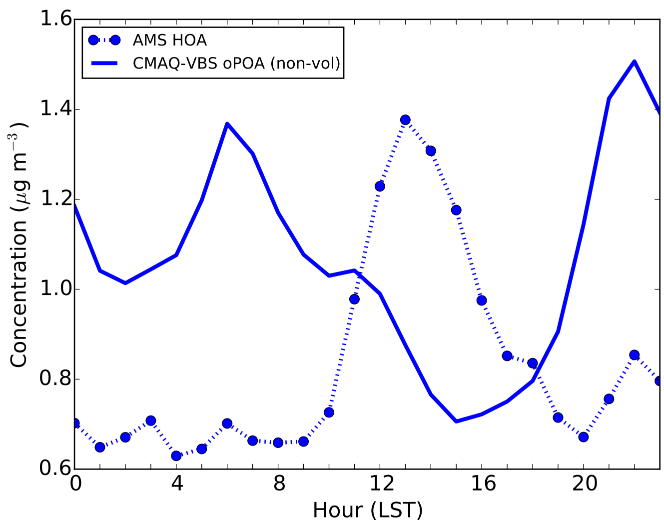


Figure S3: Diurnal profile of a nonvolatile CMAQ-VBS oPOA treatment.

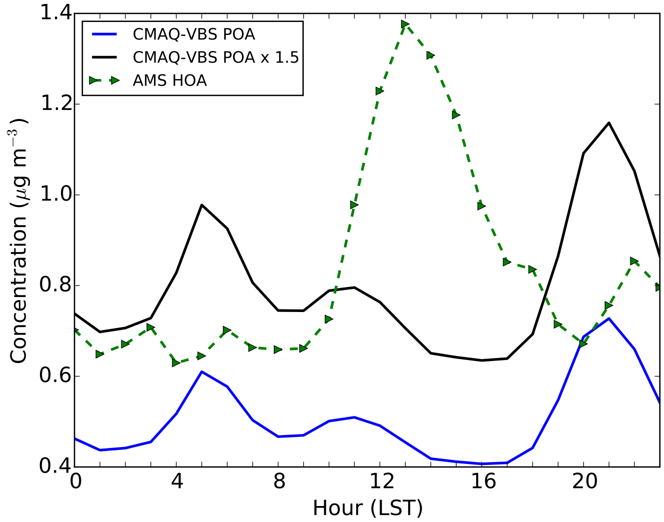


Figure S4: Diurnal profile of CMAQ-VBS oPOA, CMAQ-VBS oPOA emissions increased by 1.5, and AMS-measured HOA at Pasadena.

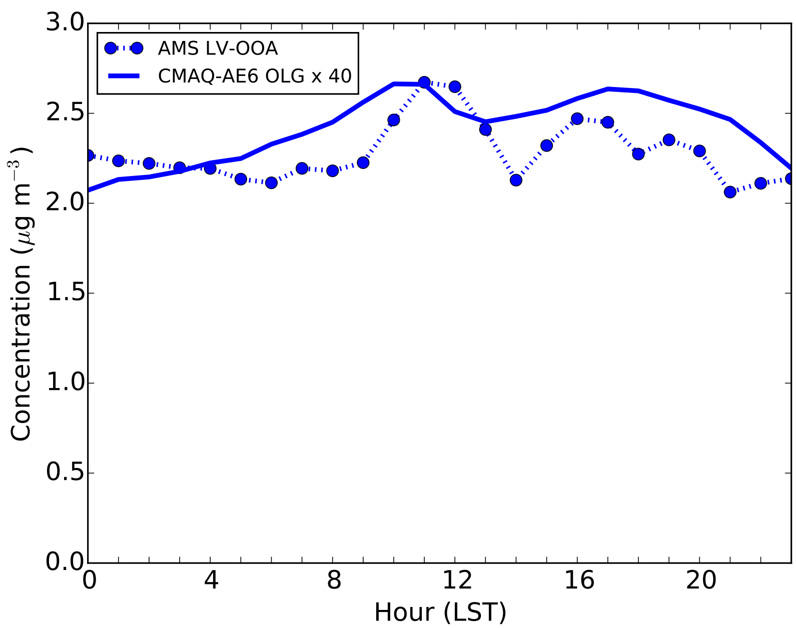


Figure S5: Diurnal profile of CMAQ-AE6 modeled SOA formed from particle oligomerization (OLG) times 40 and AMS measured LV-OOA at Pasadena.

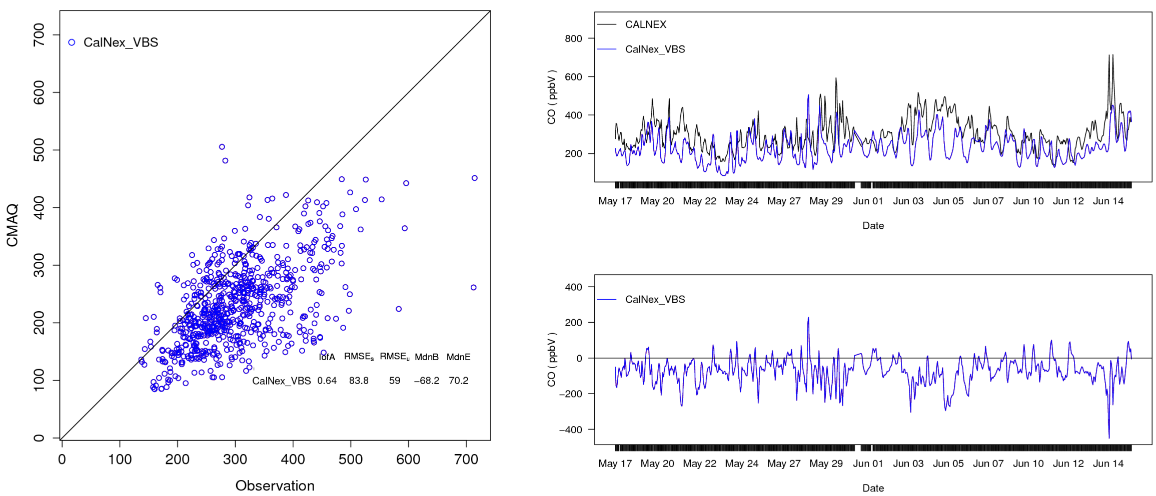


Figure S6: Comparison of CO observations at Pasadena (CALNEX) against CMAQ-VBS (CalNex_VBS) predictions (left and top right) and CMAQ-VBS model bias (bottom right).

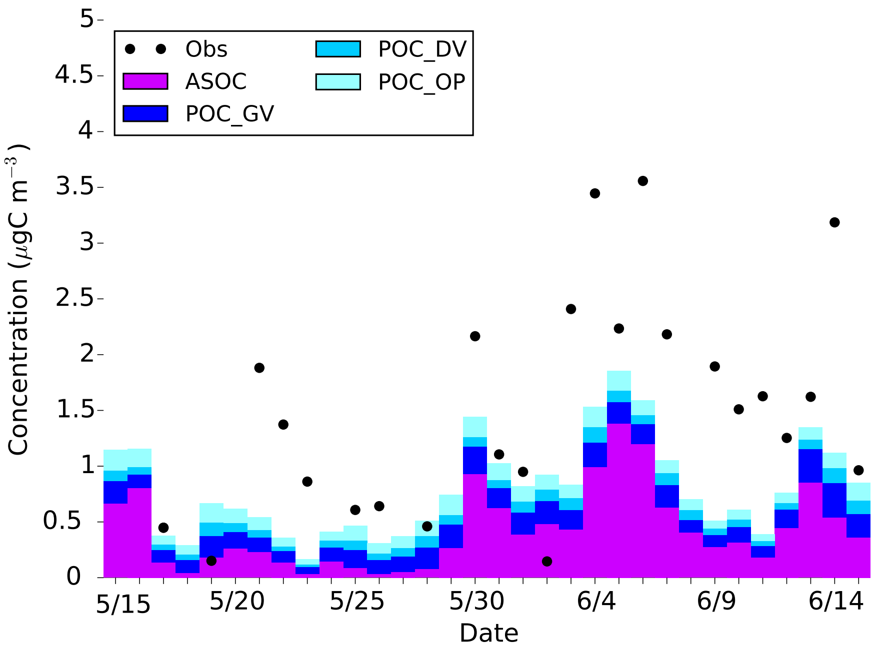
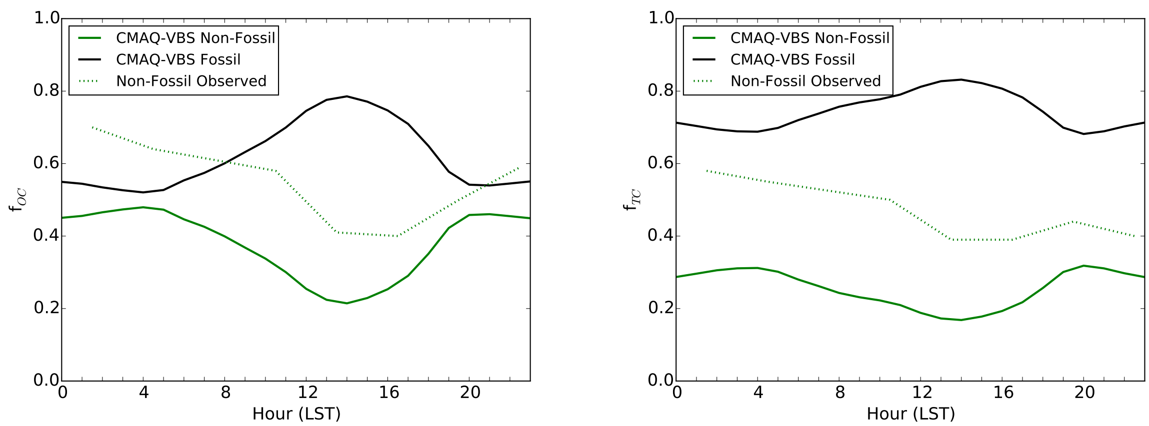


Figure S7: Daily average CMAQ-VBS non-EC fossil carbon at Pasadena. Non-EC fossil carbon model species include anthropogenic secondary OC (ASOC), and primary organic carbon from gas vehicles (POC_GV), diesel vehicles (POC_DV), and other sources (POC_OP).



(a) Fraction of OC

(b) Fraction of TC

Figure S8: CMAQ-VBS non-fossil and fossil fraction and observed non-fossil fraction from Zotter et al. (2014) for OC (a) and TC (b) at Pasadena.

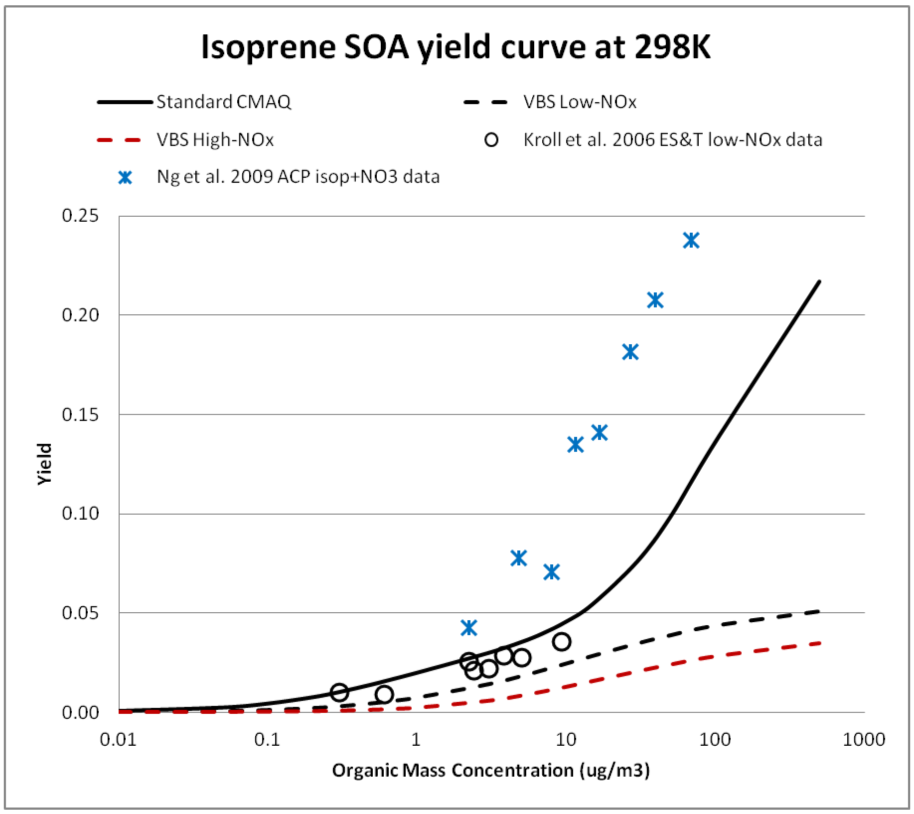


Figure S9: Isoprene SOA yield curves at the reference temperature.

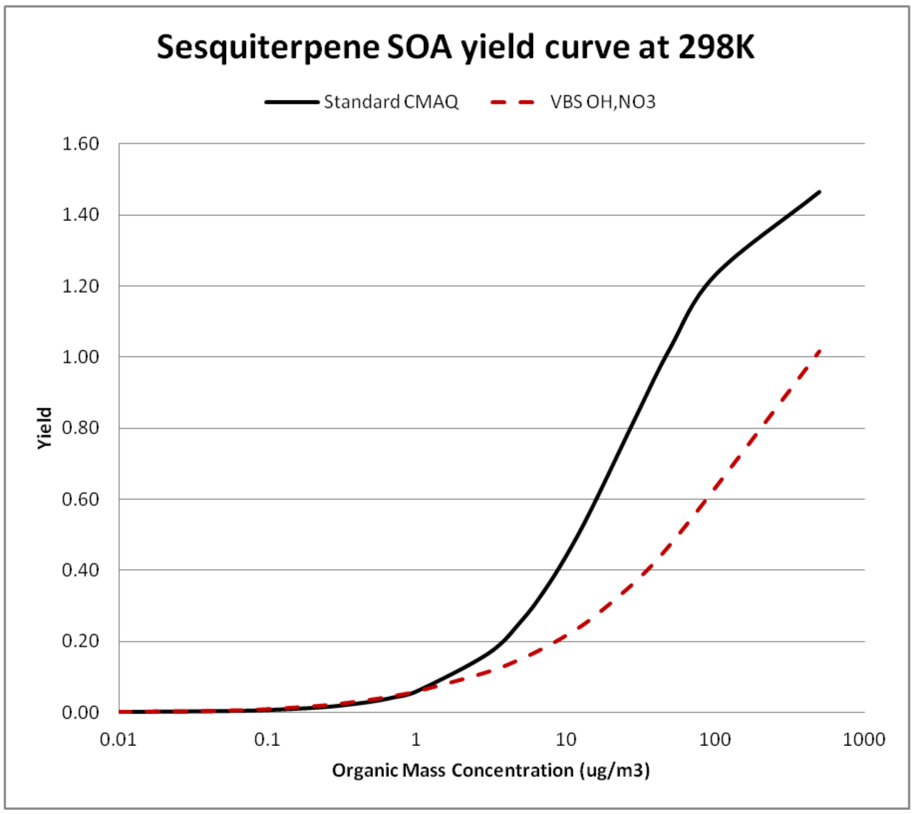


Figure S10: Sesquiterpene SOA yield curves at the reference temperature.

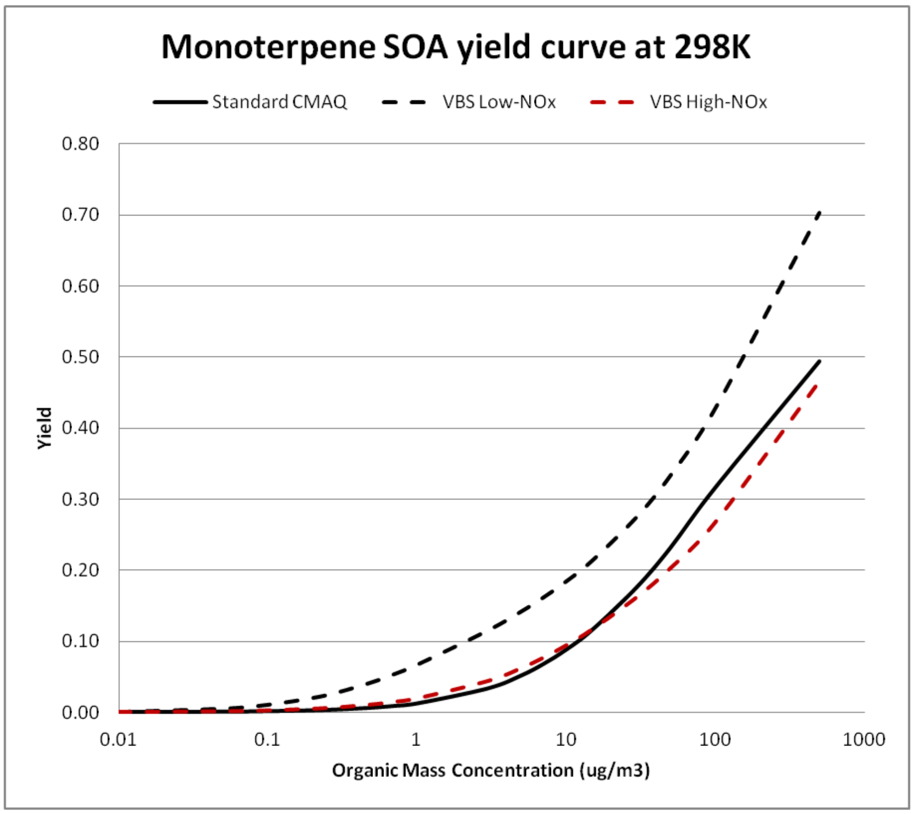


Figure S11: Monoterpene SOA yield curves at the reference temperature.

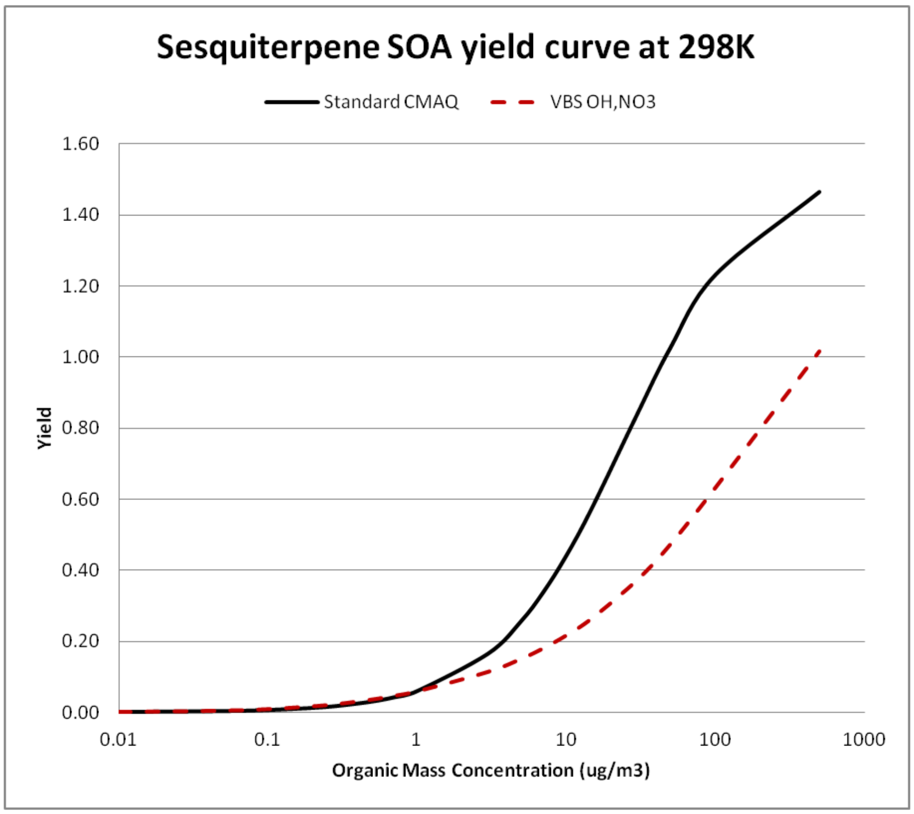


Figure S12: Sesquiterpene SOA yield curves at the reference temperature.

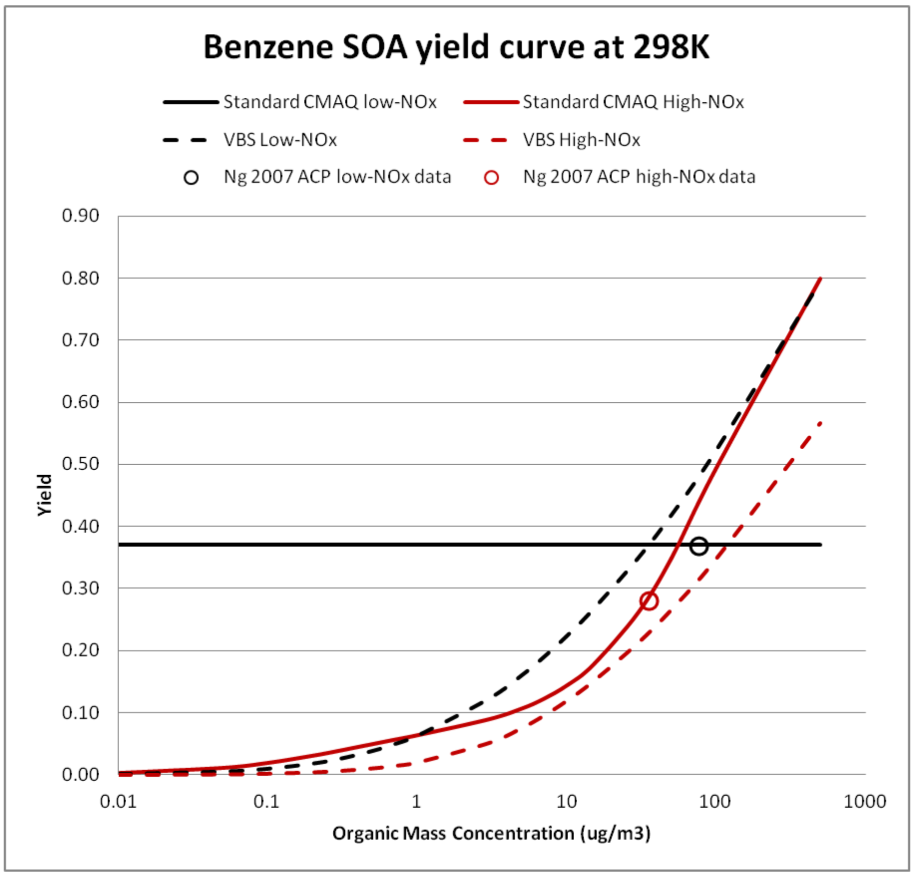


Figure S13: Benzene SOA yield curves at the reference temperature.

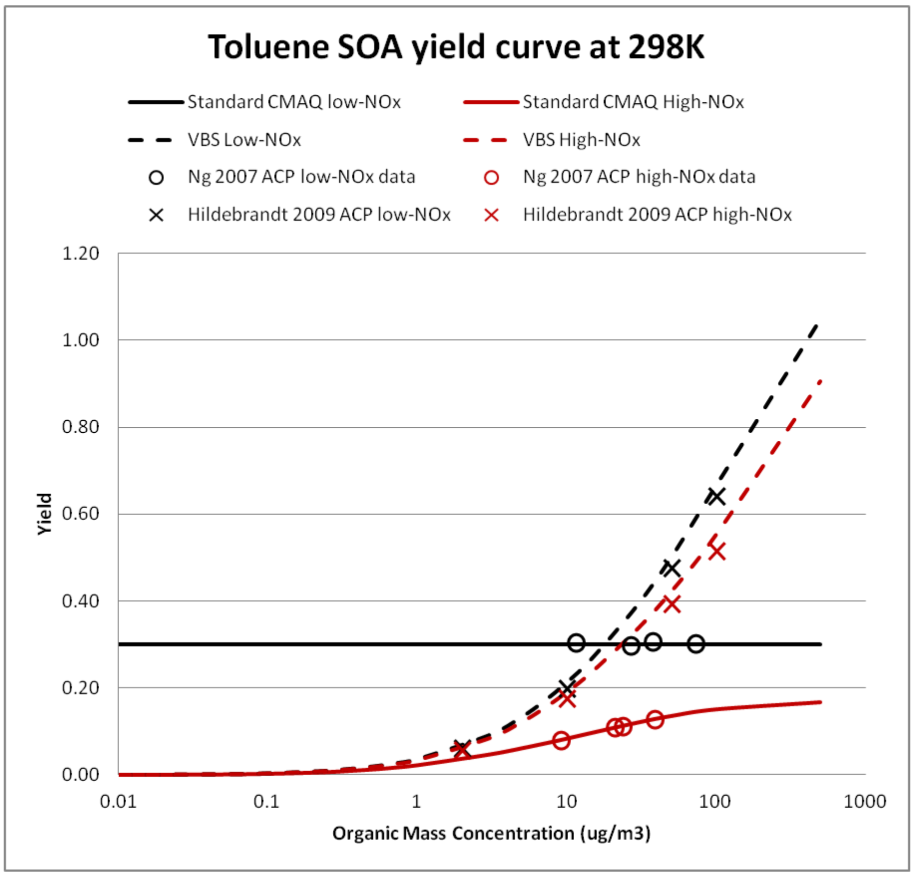
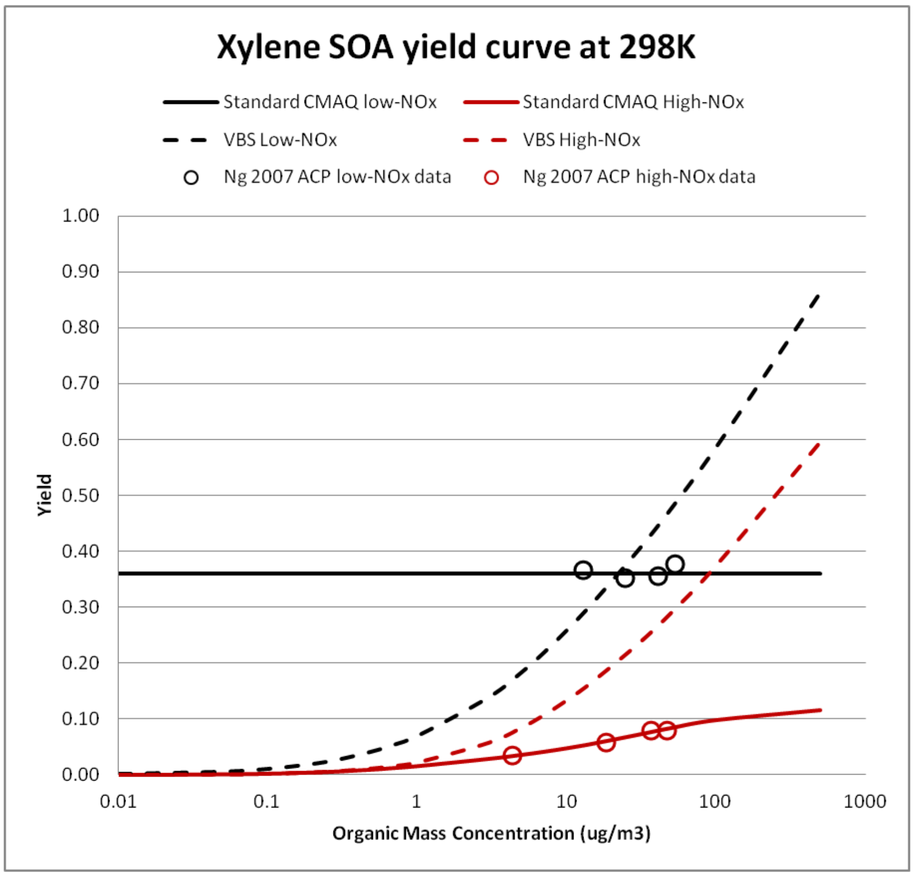


Figure S14: Toluene SOA yield curves at the reference temperature.



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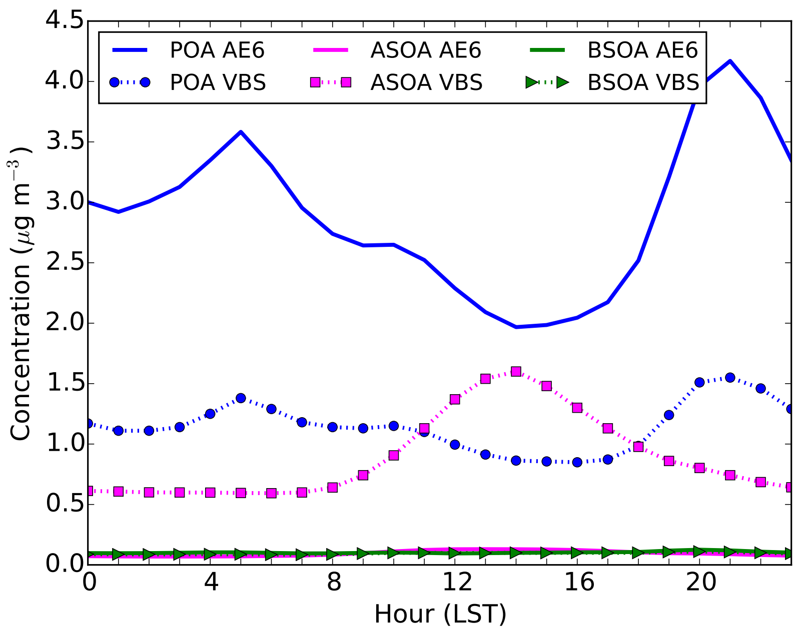


Figure S16: Comparison of the diurnal profile from CMAQ-AE6 and CMAQ-VBS predictions of primary organic aerosols (POA), anthropogenic SOA (ASOA), and biogenic SOA (BSOA) at Pasadena.

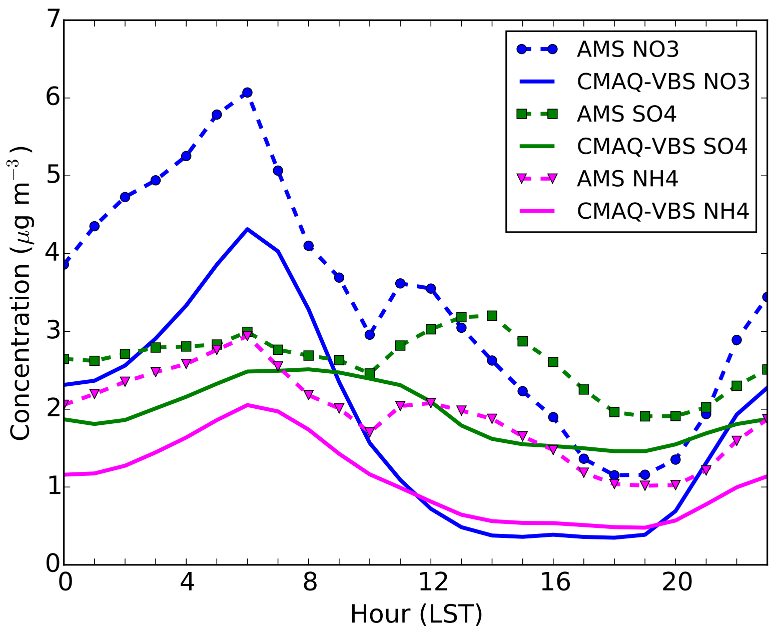
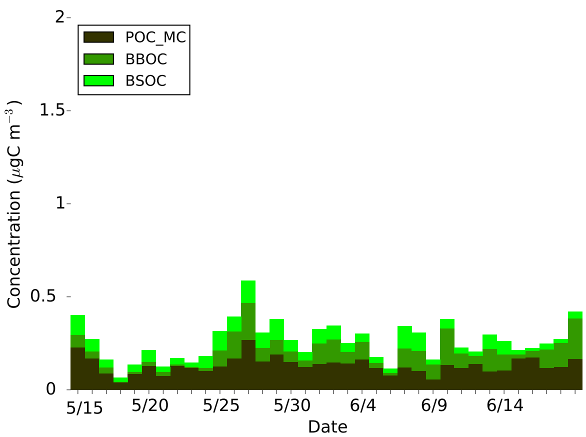
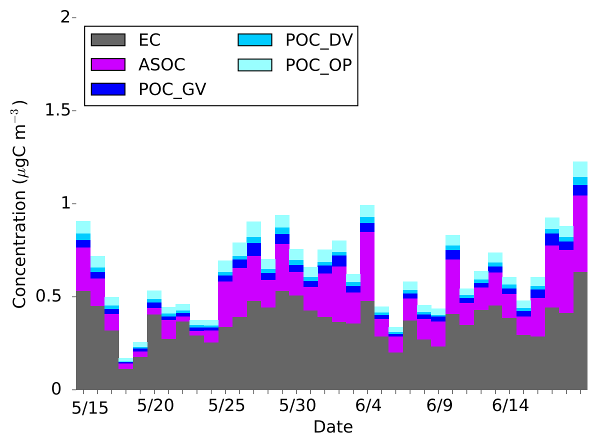


Figure S17: Comparison of AMS measured and CMAQ-VBS predicted inorganic aerosol species.

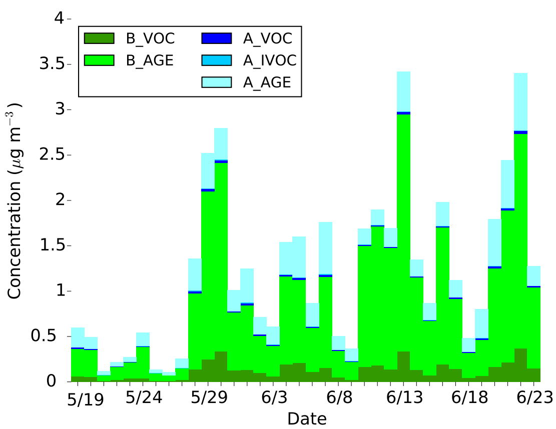


(a) Non-Fossil Carbon

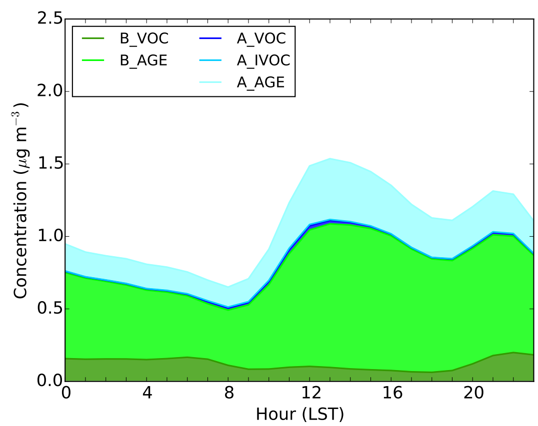


(b) Fossil Carbon

Figure S18: Daily average CMAQ-VBS non-fossil (a) and fossil (b) carbon at Bakersfield, CA. Modeled species include primary organic carbon from meat cooking (POC_MC), biomass burning OC (BBOC), biogenic secondary OC (BSOC), elemental carbon (EC), anthropogenic secondary OC (ASOC), and POC from gas vehicles (POC_GV), diesel vehicles (POC_DV), and other sources (POC_OP).



(a) Daily Average



(b) Diurnal Profile

Figure S19: Model contributions of anthropogenic and biogenic VOCs (A_VOC, B_VOC), anthropogenic and biogenic IVOCs (A_IVOC, B_IVOC), and aging reactions of anthropogenic and biogenic SOA (A_AGE, B_AGE) at Bakersfield, CA. Note aging of biogenic SOA was turned on only during sensitivity simulations.

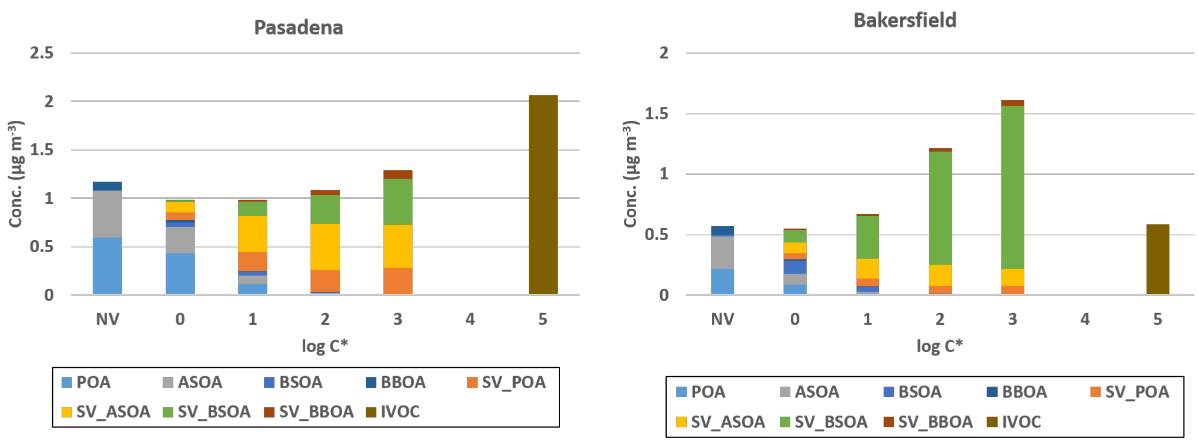


Figure S20: Volatility distribution of aerosol [primary organic aerosols (POA), anthropogenic SOA (ASOA), biogenic SOA (BSOA), and biomass burning OA (BBOA)] and semivolatile (SV_* and IVOC) CMAQ-VBS species at Pasadena and Bakersfield.

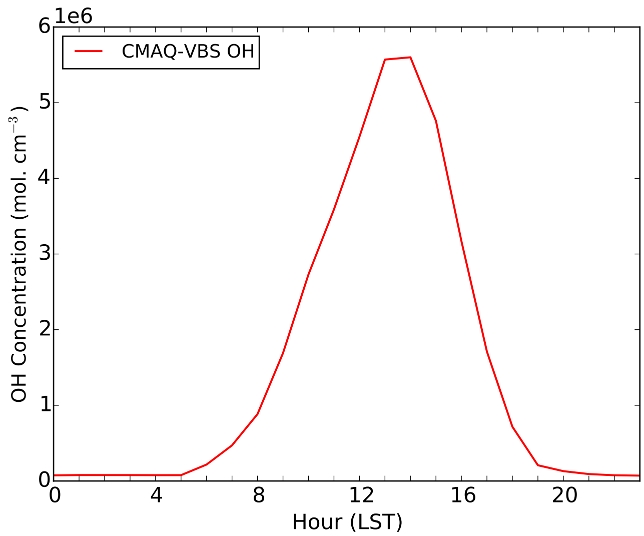


Figure S21: CMAQ-VBS modeled OH diurnal profile at Pasadena.

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Koo, B., Knipping, E., and Yarwood, G.: 1.5-Dimensional Volatility Basis Set Approach for Modeling Organic Aerosol in CAMx and CMAQ, Atmospheric Environment, 95, 158–164, 2014.