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A better representation of volatile organic compound chemistry in WRF-Chem and its impact on ozone over Los Angeles

Qindan Zhu et al.

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Species in RACM2B-VCP	Name
PROG	Propylene glycol
GLYCR	Glycerol
IPOH	Isopropanol
D4SILX	D4-Siloxane
D5SILX	D5-Siloxane
PCBTF	*p*-chlorobenzotrifluoride
PDCBZ	*p*-dichlorobenzene
ECLP	Eucalyptol

Table S1: The addition of new species in RACM2B-VCP mechanism

Reaction	Reaction coefficient	Reference
PROG+HO=0.387 ALD+0.613 HAC+HO2	2.15D-11	Coggon et al., 2021
GLYCR+HO=0.45 ALD+0.55 HKET+HO2	5.45D-11	
IPOH+HO=0.861 ACT+0.139 ACTP+0.861 HO2	ARR2(2.1D-12, -270.0_dp, TEMP)	
D4SILX+HO=ROH	1.3D-12	Alton and Browne, 2020
D5SILX+HO=ROH	2.1D-12	
PCBTF+HO=0.060 TLP1+0.763 TR2+0.177 CSL+0.177 HO2	2.5D-13	Atkinson and Arey, 2003
PDCBZ+HO=0.352 BENP+0.118 EPX+0.530 PHEN+0.648 HO2	3.2D-13	
ECLP+HO=0.951 HC8P+0.025 ALD+0.024 HKET+0.049 HO2+H2O	1.11D-11	Corchnoy and Atkinson, 1990

Table S2: The newly added reactions addressing the VOCs from VCP sources and eucalyptol to RACM2B-VCP chemical mechanism as well as their reaction coefficients.

Photolysis species in RACM-ESRL-VCP	Mapped photolysis species in TUV
pj_o31d	j_o1d
pj_o33p	j_o3p
pj_no2	j_no2
pj_hno3	j_hno3
pj_no3o2	j_no3_a
pj_no3o	j_no3_b
pj_hno4	j_hno4
pj_h2o2	j_h2o2
pj_ch3o2h	j_ch3ooh
pj_ch2or	j_ch2o_r
pj_ch2om	j_ch2o_m
pj_ch3cho	j_ch3cho_a + j_ch3cho_b + j_ch3cho_c
pj_macr	j_macr
pj_ch3coch3	j_ch3coch3
pj_ch3cocho	j_mgly
pj_ch3coc2h5	j_mek
pj_hcocho	j_gly_b
pj_hcochob	j_gly_c
pj_hchochoc	j_gly_a
pj_hno2	j_hno2
pj_ch3coo2h	j_ch3coooh
pj_hcochest	j_biacetyl
pj_ch3ono2	j_ch3ono2

Table S3: The photolysis species mapping between RACM-ESRL-VCP chemical mechanism and TUV photolysis scheme.

Photolysis species in RACM2-VCP	Mapped photolysis species in TUV
pj_o31d	j_o1d
pj_o33p	j_o3p
pj_no2	j_no2
pj_hno3	j_hno3
pj_no3o2	j_no3_a
pj_no3o	j_no3_b
pj_hno4	j_hno4
pj_h2o2	j_h2o2
pj_ch3o2h	j_ch3ooh
pj_ch2or	j_ch2o_r
pj_ch2om	j_ch2o_m
pj_ch3cho	j_ch3cho_a + j_ch3cho_b + j_ch3cho_c
pj_macr	j_macr
pj_ch3coch3	j_ch3coch3
pj_ch3cocho	j_mgly
pj_ch3coc2h5	j_mek
pj_hcocho	j_gly_b
pj_hcochob	j_gly_c
pj_hno3	j_hno2
pj_ch3coo2h	j_ch3coooh
pj_hcochest	j_biacetyl
pj_ch3ono2	j_ch3ono2
pj_ald	j_c2h5cho
pj_uald	j_acrol
pj_mvk	j_mvk
pj_hcochoc	j_gly_a
pj_bald	j_c2h5cho
pj_iprno3	j_2c4h9ono2
pj_pana	j_pan_a
pj_panb	j_pan_b
pj_hpald	j_macr
pj_glyc	j_glyald_a + j_glyald_b + j_glyald_c
pj_noa	j_ch3coch2ono2
pj_ibutald	j_ch2o_r
pj_onitOH3	j_ch2ohch2ono2
pj_onit1	j_ch2ohch2ono2
pj_onitOH1	j_ch2ohch2ono2
pj_mpn	j_ch3oono2

Table S4: The photolysis species mapping between RACM2B-VCP chemical mechanism and TUV photolysis scheme.

Reactants		Products	Rate
HPALD + hv	->	HO+HO2+0.5 HAC+0.5 MGLY+0.25 GLYC+0.25 GLY+HCHO	55*j(Pj_macr)
PROPNN+hv	->	NO2+ACO3+HCHO	j(Pj_noa)
ETHLN+hv	->	HO2+CO+HCHO+NO2	4.3*j(Pj_noa)
MACRN+hv	->	NO2+CO+HAC+HO2	5.8*j(Pj_noa)
MVKN+hv	->	GLYC+NO2+ACO3	1.26*j(Pj_noa)
ISOPNB+hv	->	ISOP+NO2	j(Pj_onitOH1)
ISOPND+hv	->	ISOP+NO2	j(Pj_onitOH1)
TONIT+hv	->	KET+NO2	j(Pj_onitOH1)
AONIT+hv	->	KET+NO2	j(Pj_onitOH1)
UTONIT+hv	->	UALD+NO2	j(Pj_onitOH1)
HONIT+hv	->	HKET+NO2	j(Pj_onitOH1)
TONIN+hv	->	KET+NO2	j(Pj_onitOH1)
UTONIN+hv	->	UALD+NO2	j(Pj_onitOH1)
IHND+hv	->	HO2+NO2+UHC+DIBOO	j(Pj_onitOH1)
IHNB+hv	->	HO2+NO2+UHC+DIBOO	j(Pj_onitOH1)
TONIH+hv	->	KET+NO2	j(Pj_onitOH1)

Table S5: The extended mapping of photolysis for species that not not included in TableS4 between RACM2B-VCP mechanism to TUV lookup table.

VOC	High NOx Conditions				Low NOx Conditions			
	1	10	100	1000	1	10	100	1000
HC5	0.0000	0.0375	0.0000	0.0000	0.0000	0.0750	0.0000	0.0000
HC8	0.0000	0.1500	0.0000	0.0000	0.0000	0.3000	0.0000	0.0000
OLT	0.0008	0.0450	0.0375	0.1500	0.0045	0.0090	0.0600	0.2250
OLI	0.0030	0.0255	0.0825	0.2700	0.0225	0.0435	0.1290	0.3750
TOL, BEN	0.0030	0.1650	0.3000	0.4350	0.0750	0.2250	0.3750	0.5250
XYL, CSL, XYO, PHEN	0.0015	0.1950	0.3000	0.4350	0.0750	0.3000	0.3750	0.5250
ISO	0.0003	0.0225	0.0150	0.0000	0.0090	0.0300	0.0150	0.0000
SESQ	0.0750	0.1500	0.7500	0.9000	0.0750	0.1500	0.7500	0.0900
API, LIM	0.0120	0.1215	0.2010	0.5070	0.1073	0.0918	0.3587	0.6075

Table S6: SOA Mass Yields for the VOC Precursors and Volatility Bins Used in WRF-CHEM for RACM2B-VCP mechanism.

Species	Gamma	Reference
ISOPNB	0.005	
TONIT	0.01	
UTONIT	0.01	Fisher et al., 2016
TONIH	0.01	
HONIT	0.01	
NO2	0.0001	
NO3	0.001	Jacob, 2000
N2O5	0.1	
HO2	0.1	Gaubert et al., 2020; Christian et al., 2017

Table S7: The summary of uptake coefficients used in RACM2B-VCP mechanisms for both inorganic nitrates and organic nitrates.

Reactions	Rates in RACM2_Berkeley 2.0	Rates in RACM2B-VCP
O3+NO=NO2{+O2}	ARR2(1.40D-12 , 1310.0_dp, TEMP)	ARR2(3.0D-12 , 1500.0_dp, TEMP)
O3+NO2=NO3{+O2}	ARR2(1.40D-13 , 2470.0_dp, TEMP)	ARR2(1.20D-13 , 2450.0_dp, TEMP)
O1D+H2O=HO+HO	2.20D-10	ARR2(1.63D-10, -60.0_dp, TEMP)
HO+M{=H2}=H2O+HO2	(5.31D-7*ARR2(7.70D-12 , 2100.0_dp, TEMP))	(5.31D-7*ARR2(2.80D-12 , 1800.0_dp, TEMP))
HO2+HO2=H2O2{+O2}	(2.2D-13*EXP(600./TEMP) + 1.90D-33* C_M *EXP(980./TEMP))	(3.0D-13*EXP(460./TEMP) + 2.10D-33* C_M *EXP(920./TEMP))
HO2+HO2+H2O=H2O2+H2O{+O2}	(3.08D-34* EXP(2800./TEMP)+ 2.59D-54* C_M *EXP(3180./TEMP))	(4.20D-34* EXP(2660./TEMP)+ 2.9D-54* C_M *EXP(3120./TEMP))
H2O2+HO=HO2+H2O	ARR2(2.90D-12 , 160.0_dp, TEMP)	1.8D-12
HO2+NO=NO2+HO	ARR2(3.60D-12 , -270.0_dp, TEMP)	ARR2(3.44D-12 , -260.0_dp, TEMP)
HO+HONO=NO2+H2O	ARR2(2.50D-12 , -260.0_dp, TEMP)	ARR2(3.0D-12 , -250.0_dp, TEMP)
O3P+NO2=NO{+O2}	ARR2(5.50D-12 , -188.0_dp, TEMP)	*ARR2(5.10D-12 , -210.0_dp, TEMP)
HO+NO2=HNO3	TROE(1.49D-30 , 1.8_dp , 2.58D-11 , 0.0_dp , TEMP, C_M)	TROE_JPL19(1.80D-30 , 3.0_dp , 2.8D-11 , 0.0_dp , TEMP, C_M)
HO2+NO3=0.3 HNO3+0.7 NO2+0.7 HO {+O2}	4.00D-12	3.50D-12
NO3+NO=NO2+NO2	ARR2(1.80D-11 , -110.0_dp , TEMP)	ARR2(1.70D-11 , -125.0_dp , TEMP)
NO3+NO2=NO+NO2{+O2}	ARR2(4.50D-14, 1260.0_dp, TEMP)	ARR2(4.35D-14, 1335.0_dp, TEMP)
NO3+NO2=N2O5	TROE(2.00D-30 , 4.4_dp , 1.40D-12 , 0.7_dp , TEMP, C_M)	TROE_JPL19(2.40D-30 , 3.0_dp , 1.60D-12 , -0.1_dp , TEMP, C_M)
N2O5=NO2+NO3	TROEE(3.70D26,11000.0_dp, 2.00D-30 , 4.4_dp , 1.40D-12 , 0.7_dp , TEMP, C_M)	TROEE_JPL19(1.72D26,10840.0_dp, 2.40D-30 , 3.0_dp , 1.60D-12 , -0.1_dp , TEMP, C_M)
HO2+NO2=HNO4	TROE(2.00D-31 , 3.4_dp , 2.90D-12 , 1.1_dp , TEMP, C_M)	TROE_JPL19(1.90D-31 , 3.4_dp , 4.0D-12 , 0.3_dp , TEMP, C_M)
HNO4=HO2+NO2	TROEE(4.76D26,10900.0_dp, 2.00D-31 , 3.4_dp , 2.90D-12 , 1.1_dp , TEMP, C_M)	TROEE_JPL19(4.76D26,10900.0_dp, 1.90D-31 , 3.4_dp , 4.00D-12 , 0.3_dp , TEMP, C_M)
HO+HNO4=NO2+H2O{+O2}	ARR2(1.30D-12 , -380.0_dp, TEMP)	ARR2(4.50D-13 , -610.0_dp, TEMP)
HO+SO2=SULF+HO2	TROE(3.30D-31 , 4.3_dp , 1.60D-12 , 0.0_dp , TEMP, C_M)	TROE_JPL19(2.90D-31 , 4.1_dp , 1.70D-12 , -0.2_dp , TEMP, C_M)

Table S8: The updates of inorganic reaction rates from RACM2_Berkeley2.0 mechanism to RACM2B-VCP mechanism.

Emission Category	Full Name	RACM_ESRL_VCP		RACM2B-VCP	
		Name	Weight	Name	Weight
CO	CO	e_co	1.00	e_co	1.00
	NO	e_no	0.90	e_no	0.90
NOX	NO2	e_no2	0.092	e_no2	0.092
	HONO	e_hono	0.008	e_hono	0.008
SO2	SO2	e_so2	1.00	e_so2	1.00
NH3	NH3	e_nh3	1.00	e_nh3	1.00
HC01	Methane	e_ch4	1.00	e_ch4	1.00
HC02	Ethane, kOH<500 /ppm/min	e_eth	1.00	e_eth	1.00
HC03	Alkane 500<kOH<2500 exclude(C3H8,C2H2,ethanol,acids)	e_hc3	1.00	e_hc3	1.00
HC04	Alkane 2500<kOH<5000 exlude(butanes)	e_hc3	1.11	e_hc3	1.11
HC05	Alkane 5000<kOH<10000 exlude(pentanes)	e_hc5	0.97	e_hc5	0.97
HC06	Alkane kOH>10000 exclude(ethylene glycol)	e_hc8	1.00	e_hc8	1.00
HC07	Ethylene	e_ol2	1.00	e_ol2	1.00
HC08	Alkene kOH <20000 /ppm/min	e_olt	1.00	e_olt	1.00
HC09	Alkene kOH >20000 /ppm/min exclude(dienes,styrenes)	e_oli	1.00	e_oli	1.00
HC10	Isoprene	e_iso	1.00	e_iso	1.00
HC11	Anthro terpenes (VCPs 7/3/19)	e_terp	1.00	e_terp	1.00
HC12	Aromatic kOH <20000 /ppm/min exclude(benzene and toluene)	e_tol	1.00	e_ben e_tol	0.50 0.50
HC13	Aromatic kOH >20000 /ppm/min exclude(xylenes)	e_xyl	1.00	e_xyl e_xyo	0.67 0.33
HC14	Formaldehyde	e_hcho	1.00	e_hcho	1.00
HC15	Acetaldehyde	e_ald	1.00	e_acd	1.00
HC16	Higher aldehydes	e_ald	1.00	e_ald	1.00
HC17	Benzaldehyde	e_ald	1.00	e_bald	1.00
HC18	Acetone	e_act	1.00	e_act	1.00
HC19	Methylethyl ketone	e_ket	1.61	e_mek	1.00
HC20	PRD2 SAPRAC species (aromatic ketones)	e_ket	1.61	e_ket	1.61
HC21	Methanol	e_moh	1.00	e_moh	1.00
HC22	Glyoxal	e_gly	1.00	e_gly	1.00
HC23	Methylglyoxal	e_mgly	1.00	e_mgly	1.00
HC24	Biacetyl	e_mgly	1.00	e_mgly	1.00
HC25	Phenols	e_csl	1.00	e_phen	1.00
HC26	Cresols	e_csl	1.00	e_csl	1.00
HC27	Methacrolein	e_macr	1.00	e_macr	1.00
HC28	Methylvinyl ketone	e_macr	1.00	e_mvk	1.00
HC29	IPRD SAPRAC species (>C4 unsaturated aldehydes)	e_ket	1.00	e_ket	1.00
HC30	Formic Acid add 1/10/2023	e_ora1	1.00	e_ora1	1.00
HC31	Acetic Acid	e_ora2	1.00	e_ora2	1.00
HC32	>C2 Acids (SAPRC PACD species)	e_ora2	1.00	e_ora2	1.00
HC33	Xylenols (SAPRC-11 species)	e_csl	1.00	e_csl	1.00
HC34	Catechols (SAPRC-11 species)	e_csl	1.00	e_mct	1.00
HC36	Propylene	e_olt	1.00	e_olt	1.00
HC37	Acetylene	e_hc3	0.40	e_ace	1.00
HC38	Benzene	e_tol	0.29	e_ben	1.00
HC39	Butanes	e_hc3	1.11	e_hc3	1.11
HC40	Pentanes	e_hc5	0.97	e_hc5	0.97
HC41	Toluene	e_tol	1.00	e_tol	1.00
HC42	m-Xylene	e_xyl	1.00	e_xyl	1.00
HC43	o-Xylene	e_xyl	1.00	e_xyo	1.00
HC44	p-Xylene	e_xyl	1.00	e_xyl	1.00
HC45	Propane	e_hc3	0.57	e_hc3	0.57
HC46	Dienes	e_oli	1.00	e_dien	1.00
HC47	Styrenes	e_olt	1.00	e_olt	1.00
HC48	Ethanol	e_eoh	1.00	e_eoh	1.00
HC49	Ethylene Glycol	e_eteg	1.00	e_eteg	1.00
PM01	Unspeciated primary PM2.5 - nuclei mode	e_pm25i	0.20	e_pm25i	0.20
	Unspeciated primary PM2.5 - accumulation mode	e_pm25j	0.80	e_pm25j	0.80
PM02	Sulfate PM2.5 - nuclei mode	e_so4i	0.20	e_so4i	0.20
	Sulfate PM2.5 - accumulation mode	e_so4j	0.80	e_so4j	0.80
PM03	Nitrate PM2.5 - nuclei mode	e_no3i	0.20	e_no3i	0.20
	Nitrate PM2.5 - accumulation mode	e_no3j	0.80	e_no3j	0.80
PM04	Organic Carbon PM2.5 - nuclei mode	e_orgi	0.20	e_orgi	0.20
	Organic Carbon PM2.5 - accumulation mode	e_orgj	0.80	e_orgj	0.80
PM05	Elemental Carbon PM2.5 - nuclei mode	e_eci	0.20	e_eci	0.20
	Elemental Carbon PM2.5 - accumulation mode	e_ecj	0.80	e_ecj	0.80
PM06	Non-Carbon Organic, PM2.5 - nuclei mode	e_orgi	0.20	e_orgi	0.20
	Non-Carbon Organic, PM2.5 - accumulation mode	e_orgj	0.80	e_orgj	0.80
PM10-PRI	Unspeciated Primary PM10	e_pm10	1.00	e_pm10	1.00
CO2	CO2	e_co2	1.00	e_co2	1.00
HC51	Isopropyl Alcohol, Oxygenated VCP add 8/2/20	e_ipoh	1.00	e_ipoh	1.00
HC52	Proplylene Glycol, Oxygenated VCP add 8/2/20	e_prog	1.00	e_prog	1.00
HC53	Glycerol, Oxygenated VCP add 8/2/20	e_glyc	1.00	e_glyc	1.00
HC54	D4-Siloxane add 8/10/22	e_tol	0.29	e_d4silx	1.00
HC55	D5-Siloxane add 8/10/22	e_tol	0.29	e_d5silx	1.00
HC56	Other Siloxane add 8/10/22	e_tol	0.29	e_ben	1.00
HC58	pcbtf add 8/10/22		1.00	e_pcbtf	1.00
HC59	pdcbz add 8/10/22		1.00	e_pdcbz	1.00

Table S9: The speciation of VOCs for both RACM-ESRL-VCP and RACM2B-VCP meachanism in the FIVE+VCP emission inventory with the addition of cooking emission.

Observations	Instrument	Species	PI
RECAP airborne	UCBerkeley PTR-TOF	VOCs: methanol, ethanol, acetaldehyde, acetone, isoprene, macr, mvk, monoterpene, benzene, toluene, benzaldehyde, xylene, d5-siloxane, PCBTF	Allen Goldstein
	UCBerkeley TD-LIF	NO, NO2	Ronald C. Cohen
	Caltch Picarro	CH4, CO	John H. Seinfeld
SUNVEx mobile	NOAA PTR-TOF-MS	VOCs: methanol, ethanol, acetaldehyde, acetone, isoprene, macr, mvk, monoterpene, benzene, toluene, benzaldehyde, xylene, d5-siloxane, PCBTF	Matthew Coggon, Chelsea Stockwell, Lu Xu, Carsten Warneke
	NOAAPicarro	CH4	Jeff Peischl
SUNVEx ground	NOAANOxCaRD	NO, NO2	Kristen Zuraski, Michael A. Robinson, Jeff Peischl, Steven. S. Brown
	NOAA CIMS	PAN	Michael A Robinson, Andy Neuman, Patrick R. Veres
	NOAA PTR-TOF-MS	VOCs: methanol, ethanol, acetaldehyde, acetone, isoprene, macr, mvk, monoterpene, benzene, toluene, benzaldehyde, xylene, d5-siloxane, PCBTF	Matthew Coggon, Chelsea Stockwell, Lu Xu, Carsten Warneke
	NOAAPicarro	CH4, CO	Jeff Peischl
	Caltch AMS	Aerosol	John H. Seinfeld

Table S10: The list of instruments and the corresponding measured species used in our study from RECAP and SUNVEx field campaigns.

Site name	Longitude	Latitude	RACM-ESRL-VCP	RACM2B-VCP
West Los Angeles	-118.46	34.05	0.05 (0.54)	0.0 (0.52)
North Main Street	-118.23	34.07	0.07 (0.77)	0.03 (0.77)
Compton	-118.2	33.90	-0.05 (0.65)	-0.09 (0.65)
Signal Hill (LBSH)	-118.17	33.79	-0.13 (0.54)	-0.17 (0.54)
Pasadena	-118.13	34.13	0.11 (0.82)	0.08 (0.83)
Pico Rivera	-118.07	34.01	0.19 (0.78)	0.15 (0.79)
La Habra	-117.95	33.92	0.27 (0.77)	0.22 (0.78)
Anaheim	-117.94	33.83	0.20 (0.73)	0.15 (0.74)
Upland	-117.63	34.10	0.21 (0.88)	0.19 (0.90)
Mira Loma (Van Buren)	-117.49	34.00	0.11 (0.89)	0.09 (0.90)
Rubidoux	-117.42	34.00	0.12 (0.87)	0.09 (0.89)
San Bernardino	-117.27	34.11	0.12 (0.87)	0.10 (0.88)

Table S11: The comparison of hourly O_3 in both WRF-Chem simulations with RACM-ESRL-VCP and RACM2B-VCP mechanism against the AQS site measurements over the study time period, including June and August 2021. For each site, we calculate the normalized mean bias (NMB) and the coefficient of determination (R^2). The R^2 is shown in the parenthesis.

Site name	Longitude	Latitude	RACM-ESRL-VCP	RACM2B-VCP
Compton	-118.2	33.90	-0.06 (0.03)	-0.07 (0.03)
Signal Hill (LBSH)	-118.17	33.79	-0.23 (0.08)	-0.23 (0.09)
Anaheim	-117.94	33.83	-0.17 (0.13)	-0.19 (0.15)
Ontario	-117.62	34.03	-0.20 (0.18)	-0.17 (0.22)
Rubidoux	-117.42	34.00	-0.08 (0.23)	-0.09 (0.24)

Table S12: The comparison of hourly $PM_{2.5}$ in both WRF-Chem simulations with RACM-ESRL-VCP and RACM2B-VCP mechanism against the AQS site measurements over the study time period, including June and August 2021. For each site, we calculate the normalized mean bias (NMB) and the coefficient of determination (R^2). The R^2 is shown in the parenthesis.

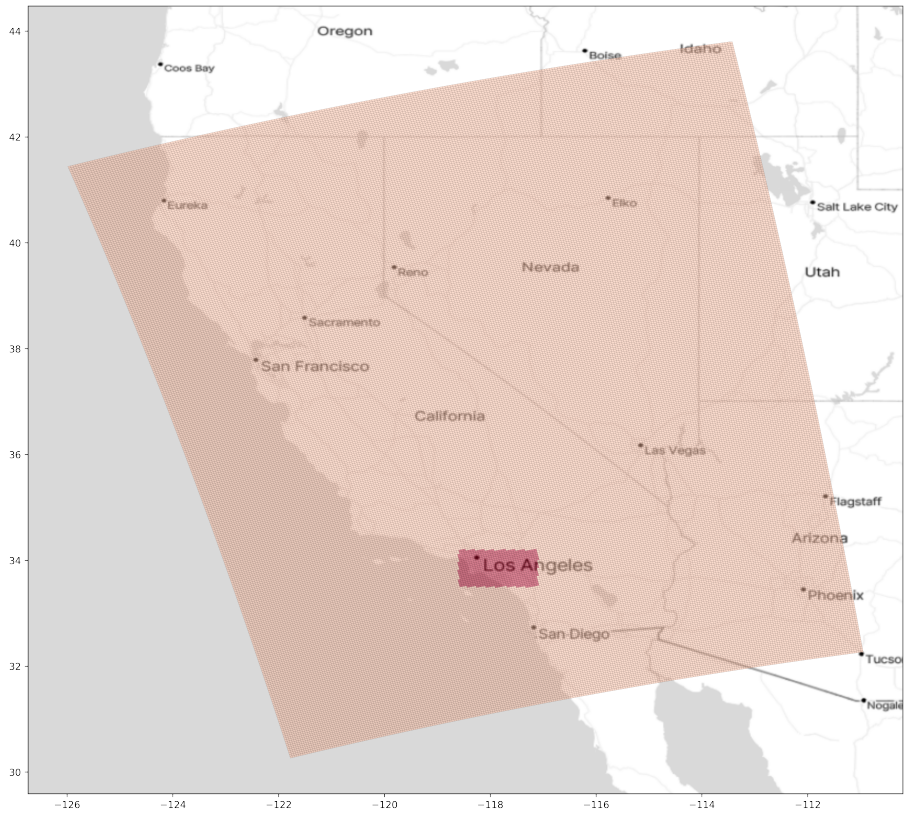

Figure S1: The model domain defined in our WRF-Chem simulation at the spatial resolution of 4km, and the region in red denotes the LA domain used in our analysis.

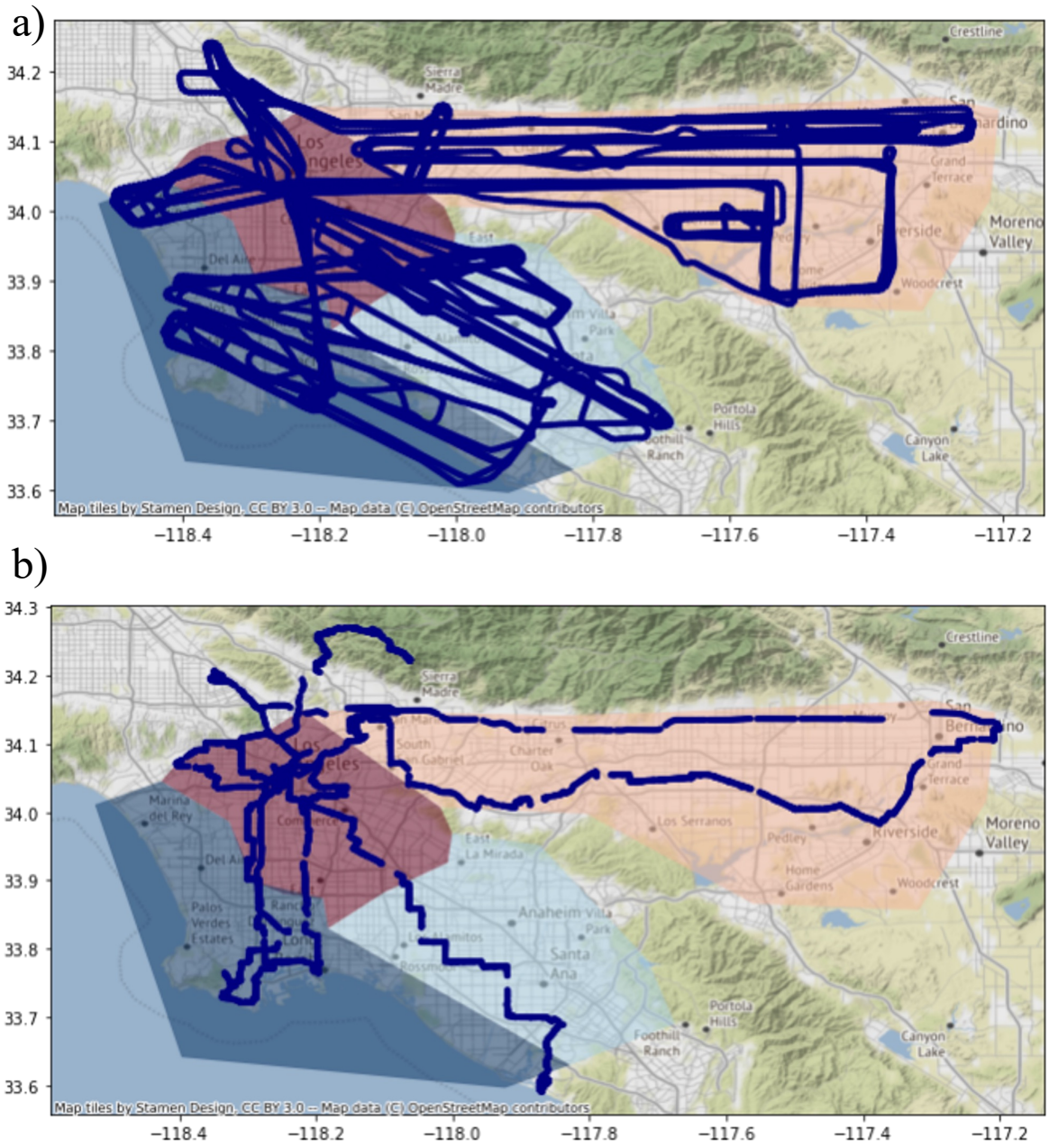

Figure S2: a) the flight track for 9 flights during RECAP-CA field campaign; b) the track of 8 days mobile laboratory by NOAA CSL during SUNVEx field campaign. Both flight and mobile tracks are categorized into four regions in colored shades: Downtown LA (red), San Bernadino Valley (pink), Santa Ana Valley (light blue), and Coastal LA (dark blue).

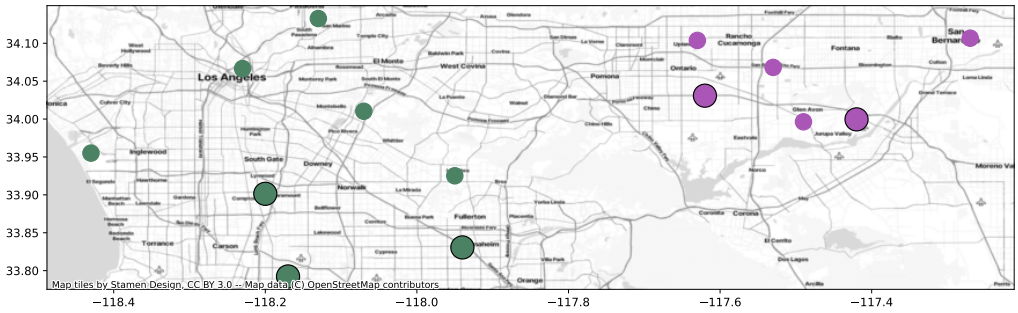

Figure S3: The map of AQS sites with available O_3 and $PM_{2.5}$ observations. The sites in green are in the region categorized as West/Central LA, and the sites in purple are in the region categorized as East Basin. Ozone observations are available for all sites, and the $PM_{2.5}$ observations are only available in sites marked with larger size and black edge colors.

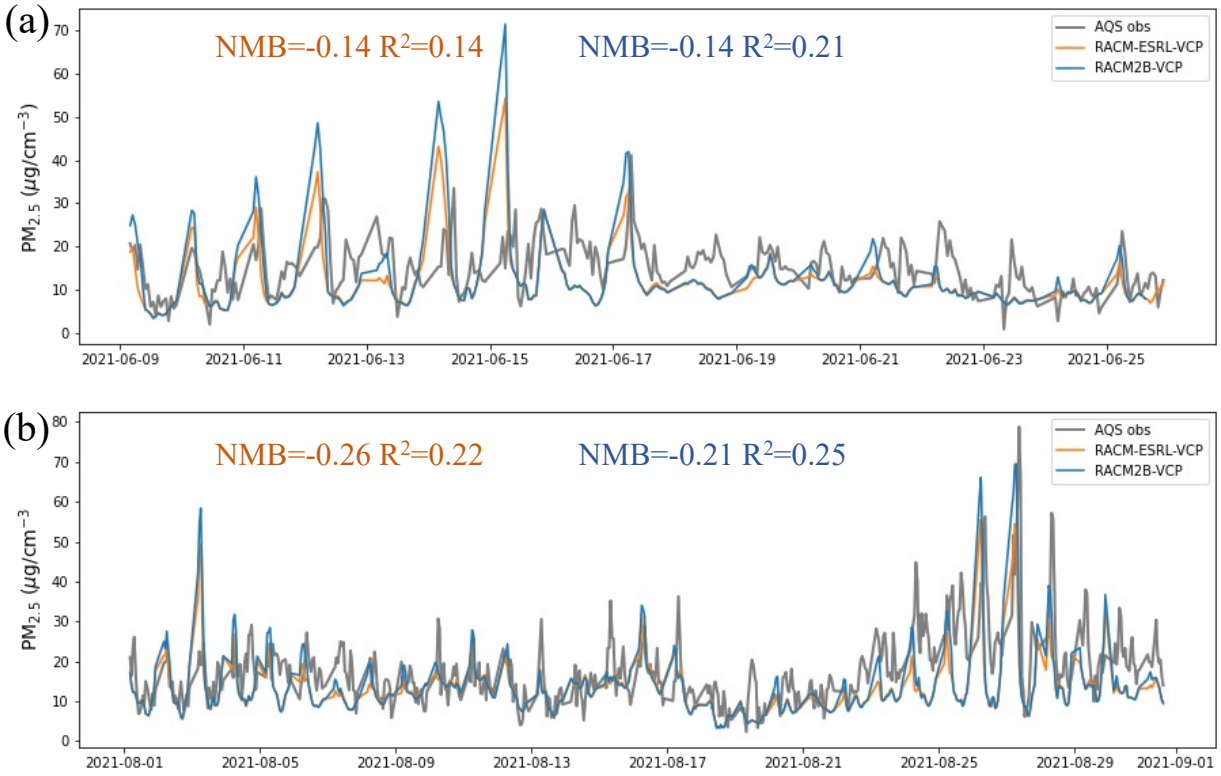

Figure S4: The comparison of time series of hourly $PM_{2.5}$ between AQS site and two WRF-Chem simulations, one with RACM-ESRL-VCP and another one with RACM2B-VCP chemical mechanism at AQS site at Ontario site (-117.62° longitude, 34.03° latitude). The corresponding R^2 between model simulations and observations of hourly $PM_{2.5}$ is shown on each plot.

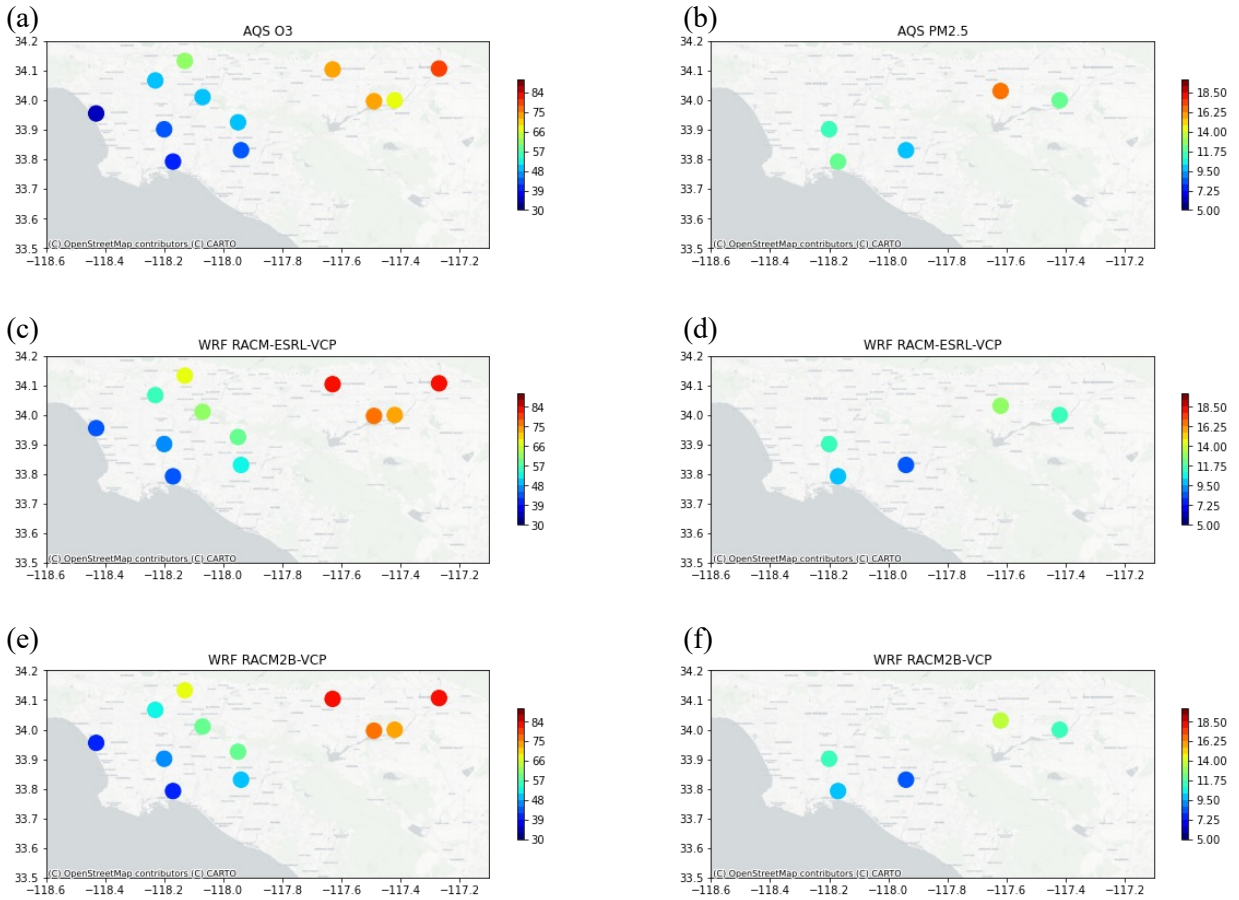

Figure S5: The map of MDA8 O_3 and daily $PM_{2.5}$ averaged over the study period from observations (a and b), from WRF-Chem simulation with RACM-ESRL-VCP chemical mechanism (c and d), and from WRF-Chem simulation with RACM2B-VCP chemical mechanism (e and f).

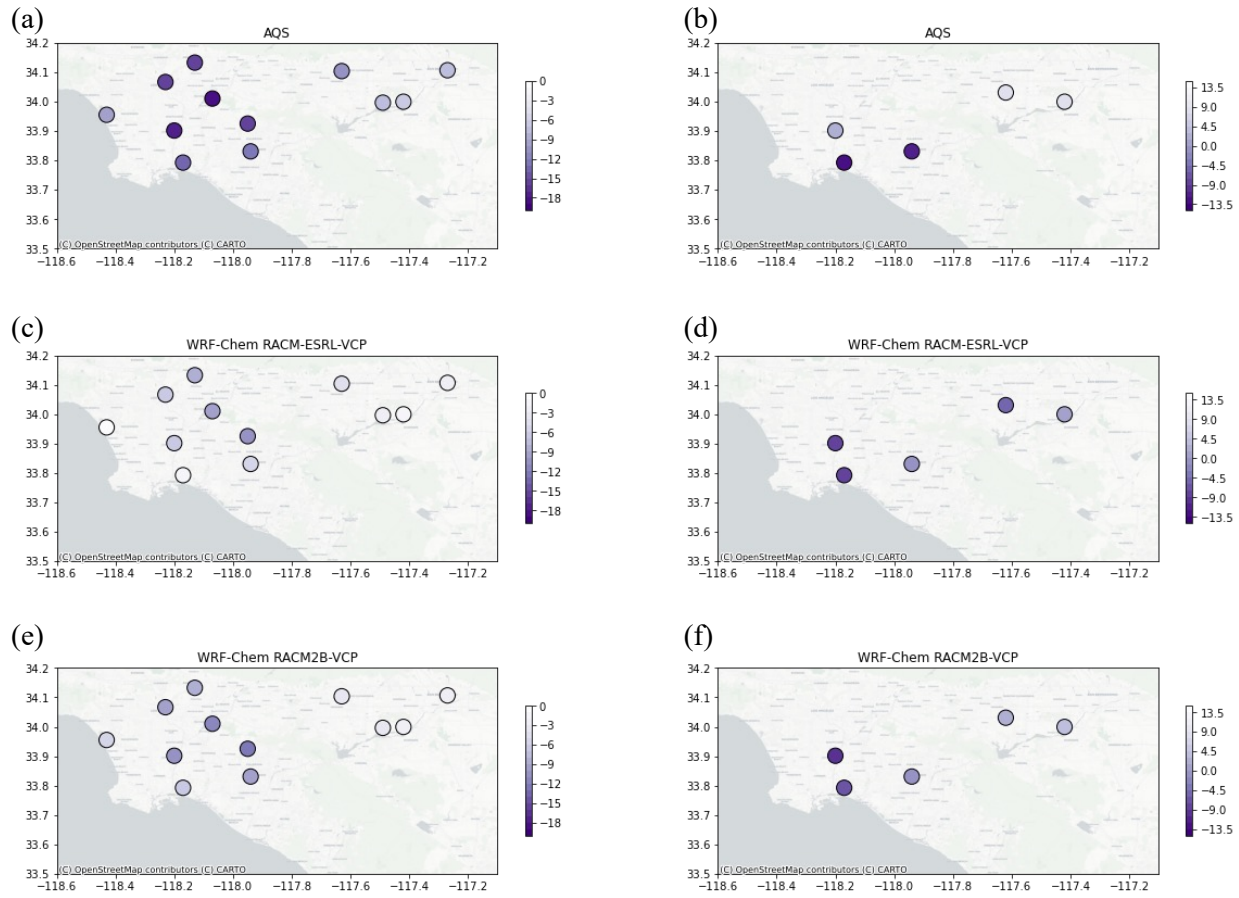

Figure S6: The map of the weekday-weekend difference relative to the average of MDA8 O_3 (Δ MDA8 O_3) and daily $PM_{2.5}$ from observations (a and b), from WRF-Chem simulation with RACM-ESRL-VCP chemical mechanism (c and d), and from WRF-Chem simulation with RACM2B-VCP chemical mechanism (e and f).

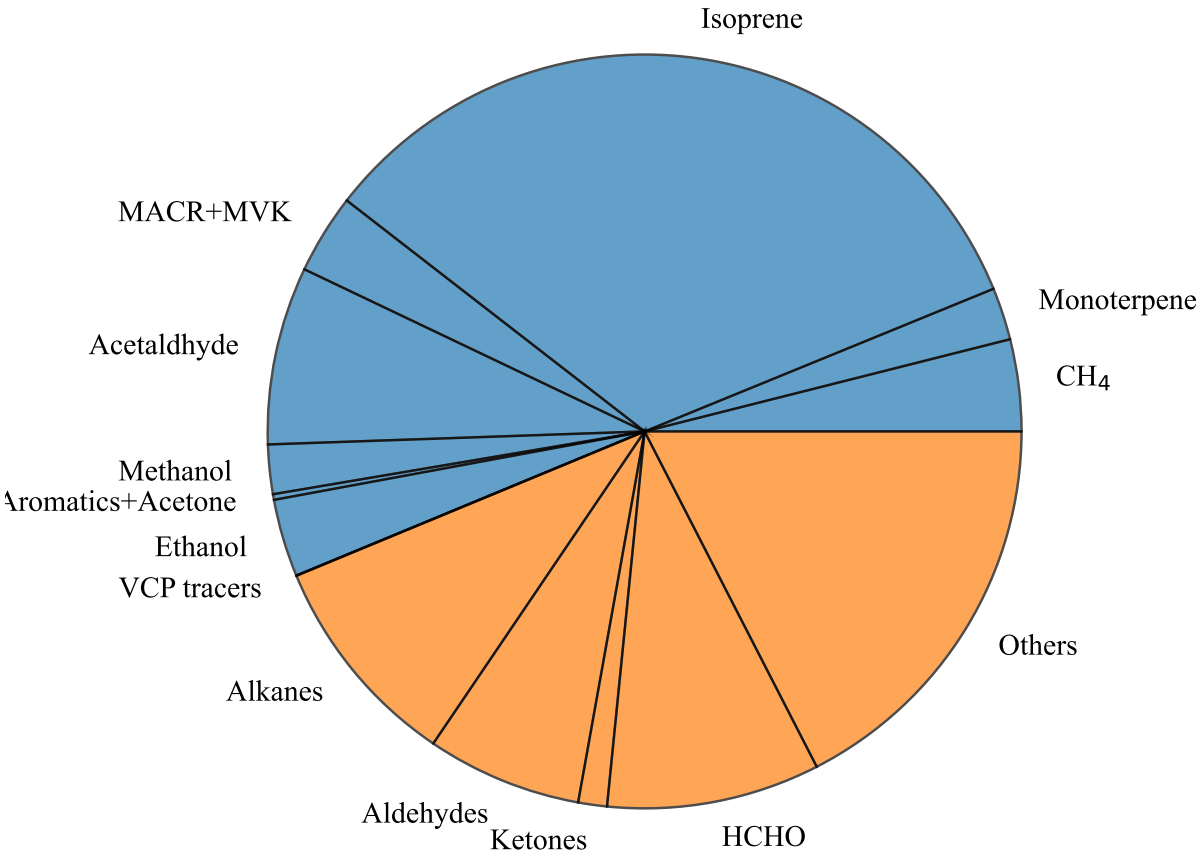

Figure S7: The budget of total surface VOC reactivity averaged over the LA region during the time period. The contributions from VOC species that are measured and calibrated during RECAP and SUNVEx field campaigns are shown in blue, and the contributions from other VOC species are shown in orange.

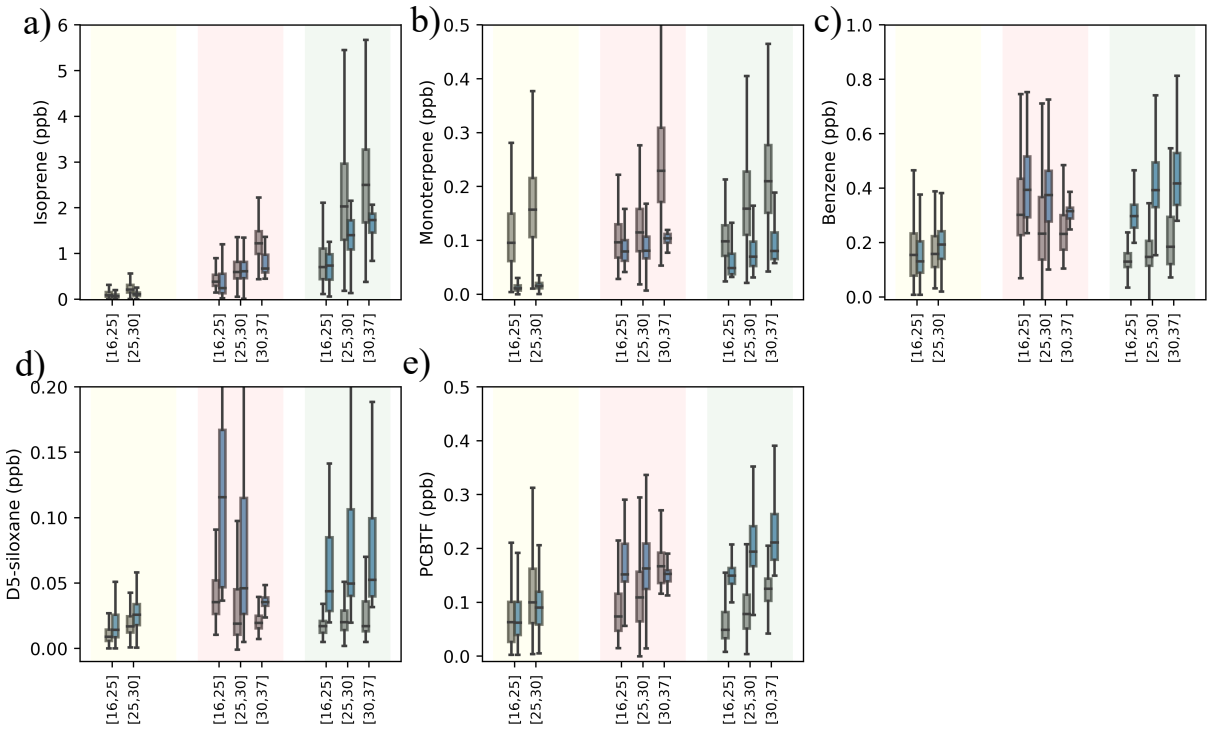

Figure S8: The comparison of the temperature dependence of key VOCs, including isoprene, monoterpene, benzene, D5-siloxane, and PCBTF, between observations (gray) and WRF-Chem simulation configured with RACM2B-VCP chemical mechanism (blue). The comparison to the RECAP airborne measurement in yellow shade; SUNVEX mobile measurements in red shade and SUNVEX ground measurements in green shade. The distribution is shown by a whisker plot; the line denotes the median value.

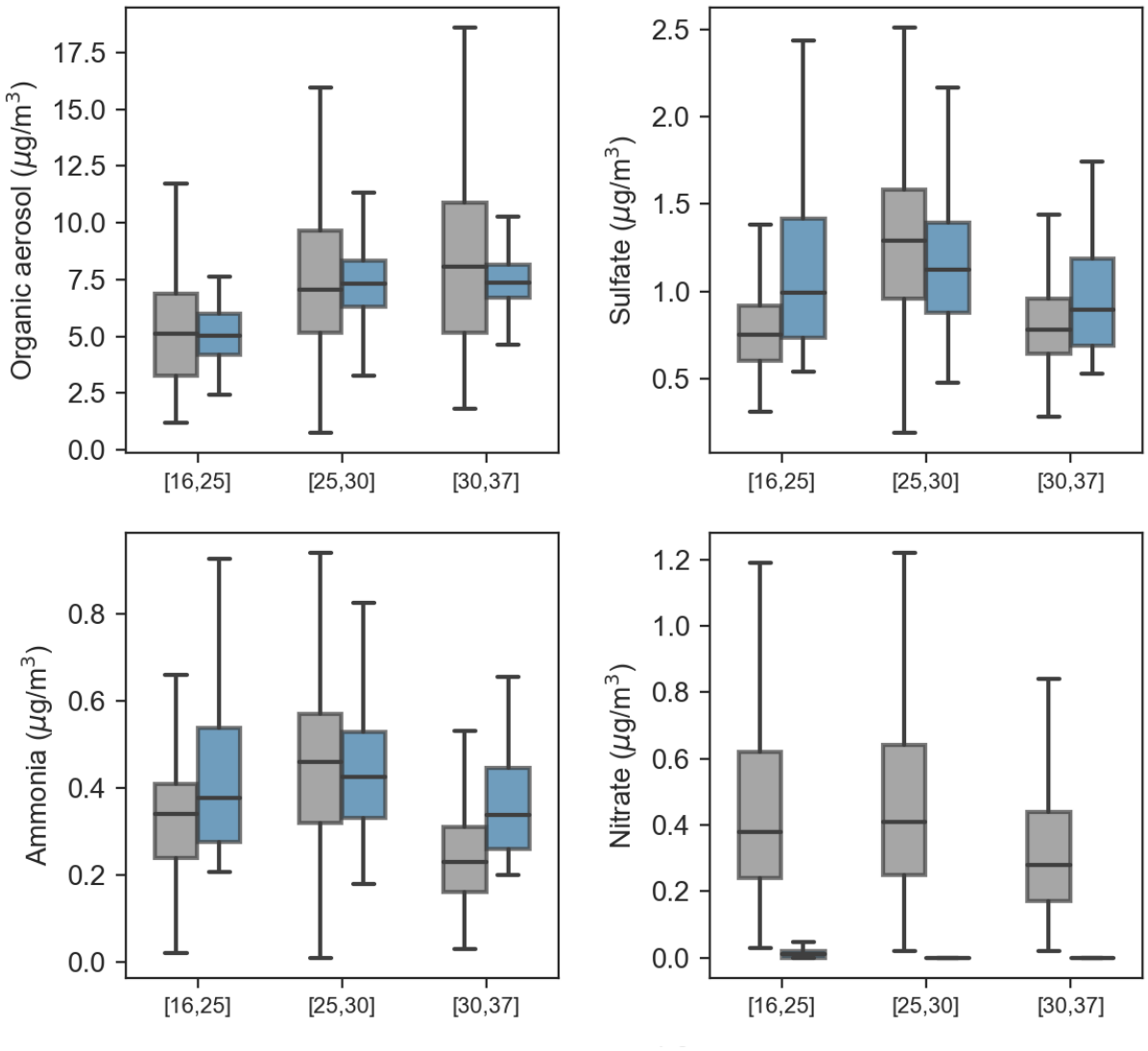

Figure S9: The comparison of the temperature dependence of aerosols, including organic, sulfate, ammonium, and nitrate aerosols, between in-situ observations (gray) and WRF-Chem simulation configured with RACM2B-VCP chemical mechanism (blue) at Pasadena. The distribution is shown by a whisker plot; the line denotes the median value.

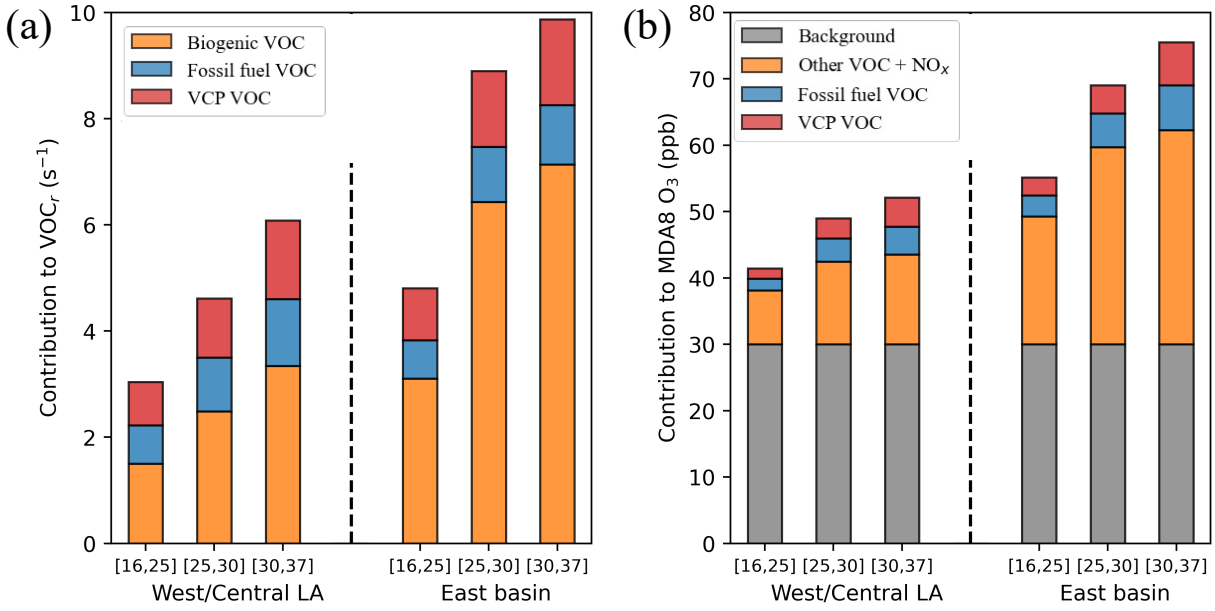

Figure S10: The contribution of VOC emissions from VCP and fossil fuel sources to VOC reactivity (a) and MDA8 O_3 (b), in West/Central LA and in East basin, under three temperature bins.

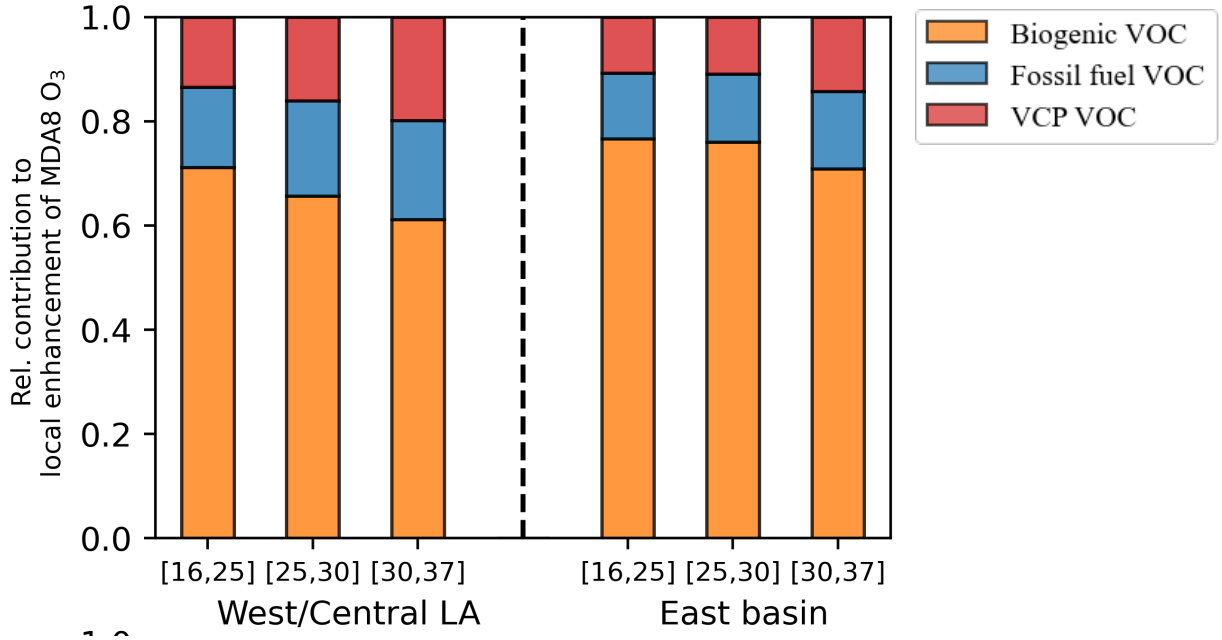

Figure S11: The relative contribution of VOC emissions from VCP and fossil fuel sources to local enhancement of MDA8 O_3 in West/Central LA and in East basin, under three temperature bins.