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Supplement of

PAMS-constrained top-down calibration of VOC-speciated CMAQ simulations

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Figures S1 to S5

Tables S1 to S5

Additional text

It is noted that, in the model, the VOC speciation is based on the U.S. Source Classification Code (SCC) profiling (SPECIATE 4.5 database issued by the U.S. EPA), which is not necessarily applicable to other regions such as Taiwan. Even this database in the U.S. needs to be constantly updated (Ying and Li, 2011). For instance, Chen et al. (2010) pointed out the difference in household VOC profiling between the U.S. and Taiwan. The household fuel used in the U.S. is mainly methane in natural gas, but in addition to natural gas used in major metropolises, it is mostly LPG, composed mainly of *propane* and *butane*, used in wider areas of Taiwan. The VOC profiles assigned for households in Taiwan are **External Combustion Boiler – Natural Gas** (0003) and **Residential Fuel – Natural Gas** (0195). While the 0195 profile is 100% methane, the 0003 profile has 56% methane and only 4% propane (**Fig. S5**). As a result, the 0003 profile is not suitable for households in Taiwan (propane should be given a higher emission factor than methane).

Other major sources could encounter similar profiling errors. Another deficiency is the lack of profiles. For instance, the default profile (Overall Average, 0000) is commonly assigned to sources without corresponding SCC profiles. Taking the top 10 emission entries with high ozone formation potentials (OFPs) in a major metropolis of Taiwan (Taoyuan City with a population of 2 million) as an example, the inventory registers seven facility types, consisting of Textile Finishing (1140), Printing Service (1602), Plastic Products (2209), Integrated Circuits (2611), Other General-purpose Machinery (2939), Motor Vehicle Manufacture (3010), and Other Manufacturing Not Elsewhere Classified (3399). However, these seven industry types have no corresponding SCC profiles and thus are all being assigned as the default profile. This issue is not unique to Taiwan but is common in the U.S too. The U.S. EPA may have continued to update the database by replacing the default profile with more appropriate source profiles. For instance, in SPECIATE 4.5, 80% of the Pulp and Paper facility type is reassigned from profiles No. 0000 and 1185 to 63 separated profiles, and 22% of the Chemical Manufacturing facility type is reassigned from profile No. 0000 to 15 separated profiles (Strum et al., 2017). In other words, every time the emission inventory gets updated, the assignment of VOC profiles should also be re-examined and revised accordingly to perform more accurate OFP estimates.

It should be noted that unrealistic VOC profiling in the inventory may not be critical if ozone simulation is the aim. However, it can be error-prone if the sources with high OFPs of individual species are to be sought. Establishing localized speciation profiles for VOCs from key emission sources is crucial for accurately calculating OFPs and informing realistic ozone control policymaking through modeling. This approach enables the identification of key VOC species or specific sources, as outlined in the Selective Precursor Mitigation (SPM) concept (Chen et al., 2024).

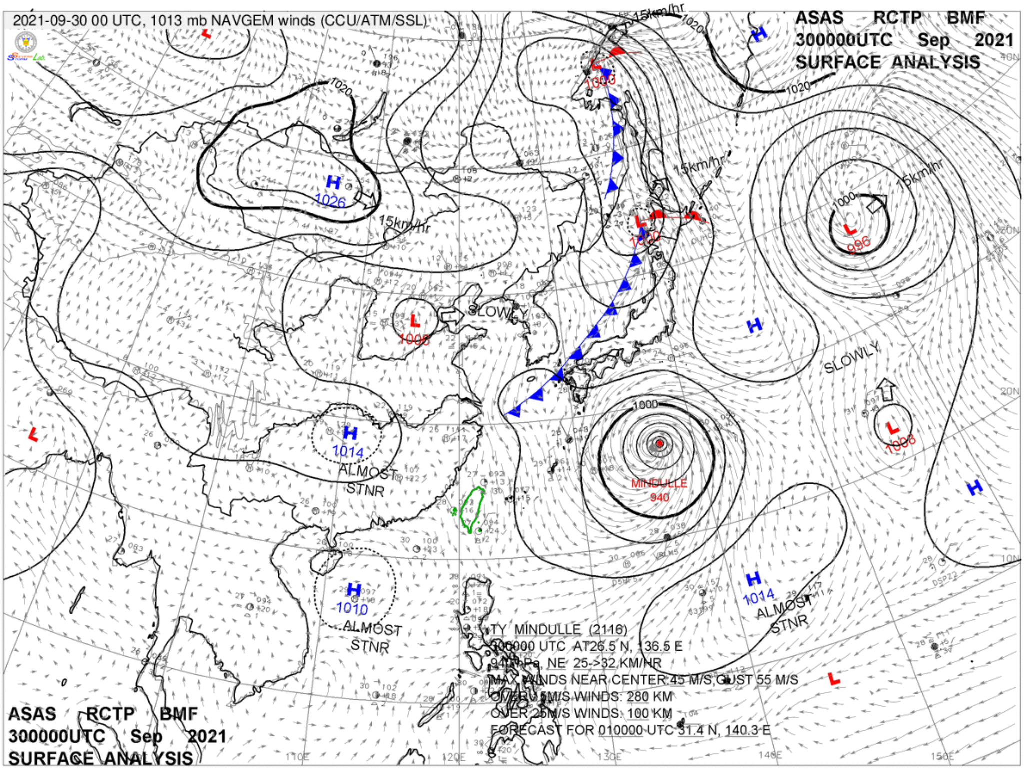


Fig. S1. Synoptic weather patterns in East Asia for the selected case in 2021.

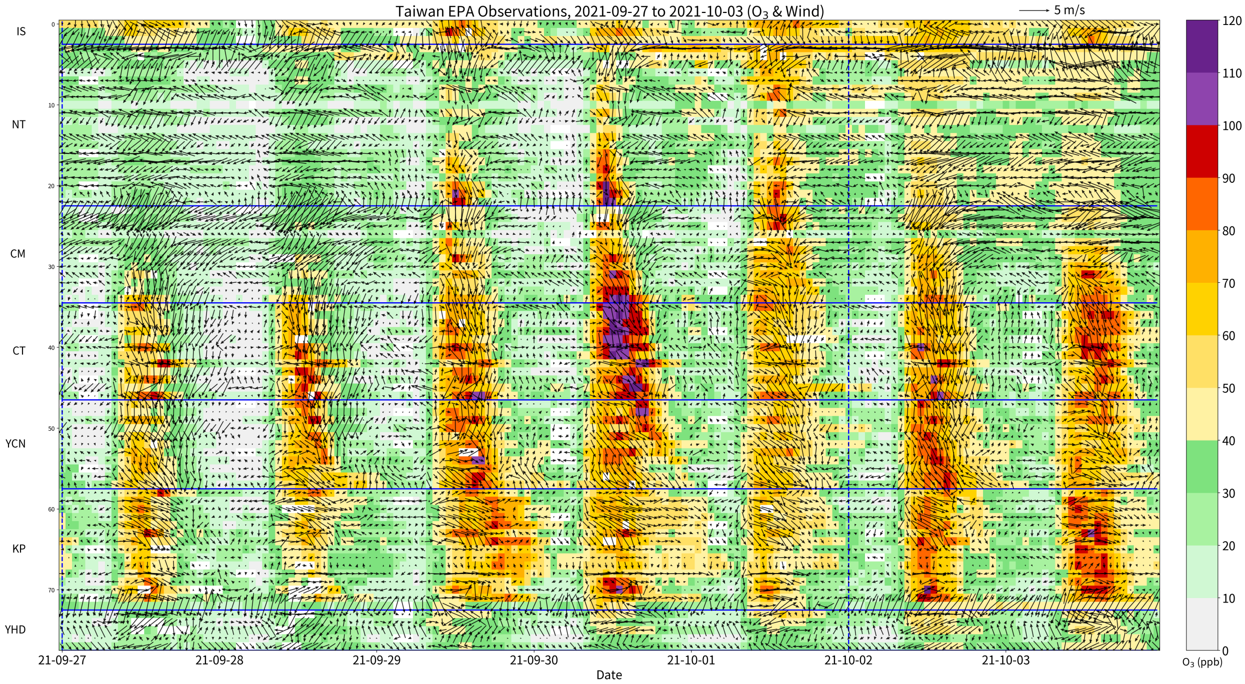
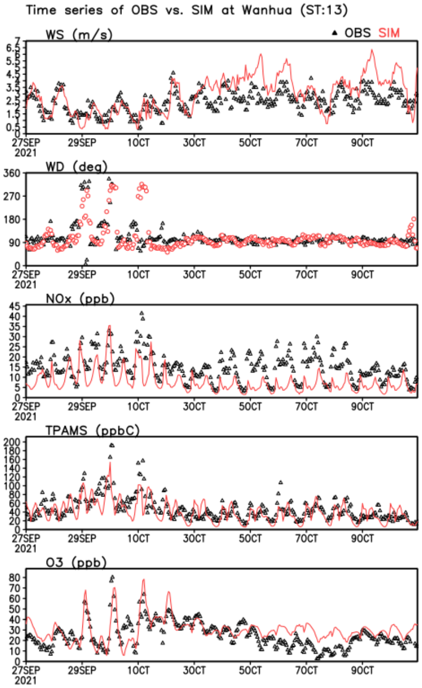
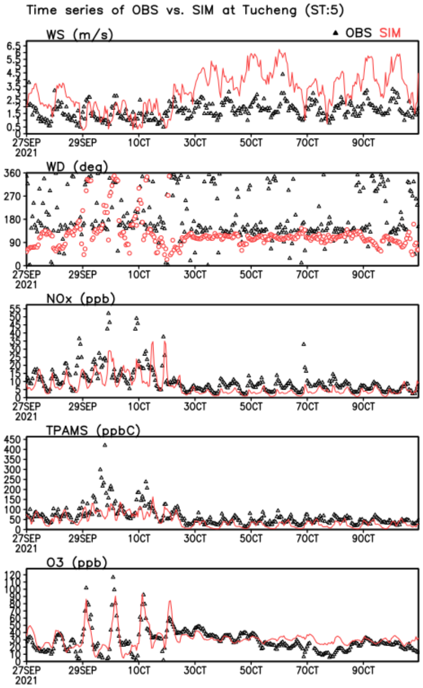
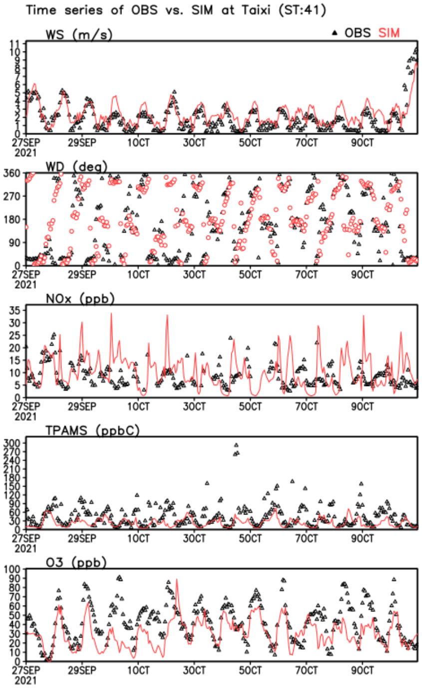
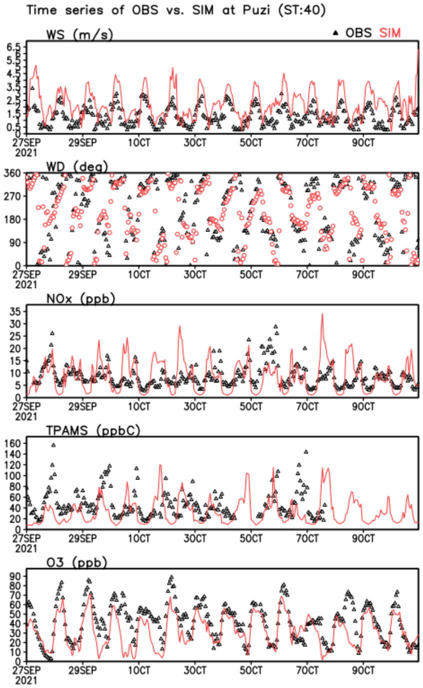


Fig. S2. Hourly observations of O_3 and horizontal surface wind vectors (10m) at all AQS from north to south of Taiwan (IS→NT→CM→CT→YCN→KP→YHD) for the selected case in 2021 (2021/09/27-10/10). The y-axis indicates station sequence, not altitude.


Time series of OBS vs. SIM at Wanhua (ST:13)
WS (m/s)
▲ OBS SIM
WD (deg)
NOx (ppb)
TPAMS (ppbC)
O3 (ppb)
27SEP
2021
29SEP
1OCT
3OCT
5OCT
7OCT
9OCT


Time series of OBS vs. SIM at Tucheng (ST:5)
WS (m/s)
▲ OBS SIM
WD (deg)
NOx (ppb)
TPAMS (ppbC)
O3 (ppb)
27SEP
2021
29SEP
1OCT
3OCT
5OCT
7OCT
9OCT


Time series of OBS vs. SIM at Taixi (ST:41)
WS (m/s)
▲ OBS SIM
WD (deg)
NOx (ppb)
TPAMS (ppbC)
O3 (ppb)
27SEP
2021
29SEP
1OCT
3OCT
5OCT
7OCT
9OCT


Time series of OBS vs. SIM at Puzi (ST:40)
WS (m/s)
▲ OBS SIM
WD (deg)
NOx (ppb)
TPAMS (ppbC)
O3 (ppb)
27SEP
2021
29SEP
1OCT
3OCT
5OCT
7OCT
9OCT

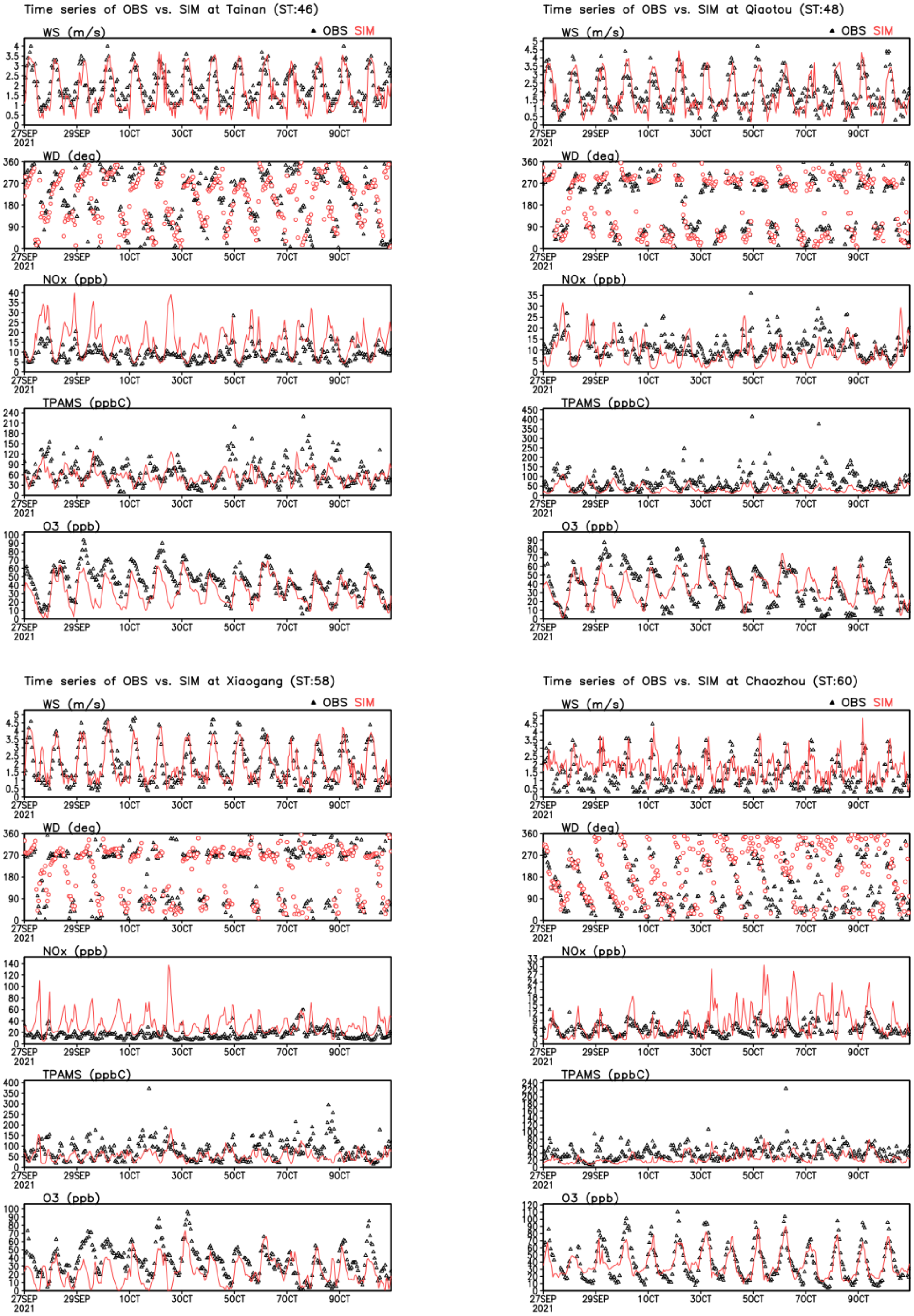
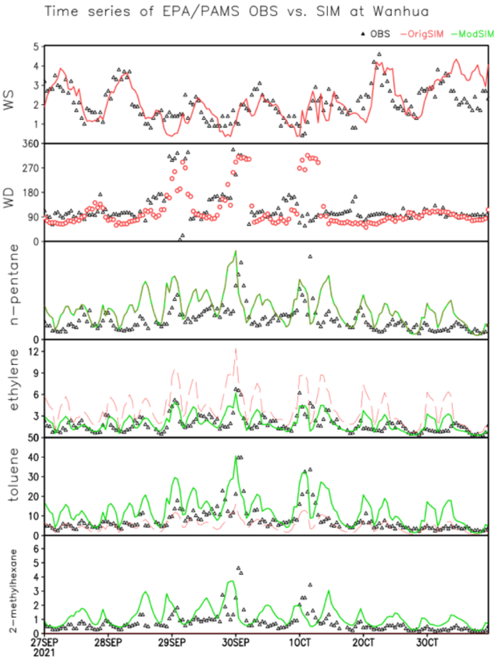
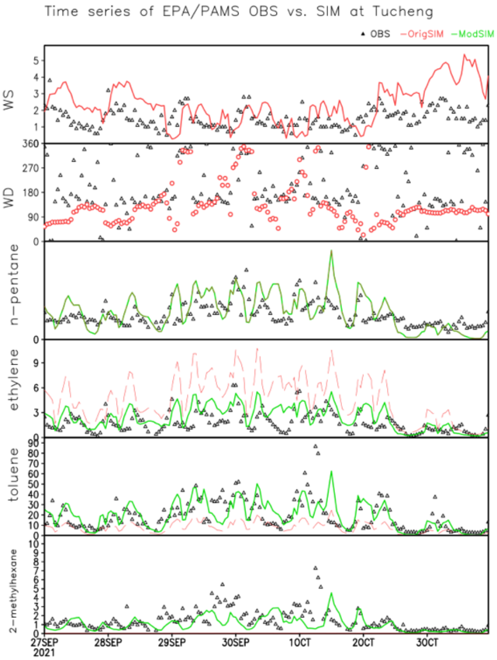
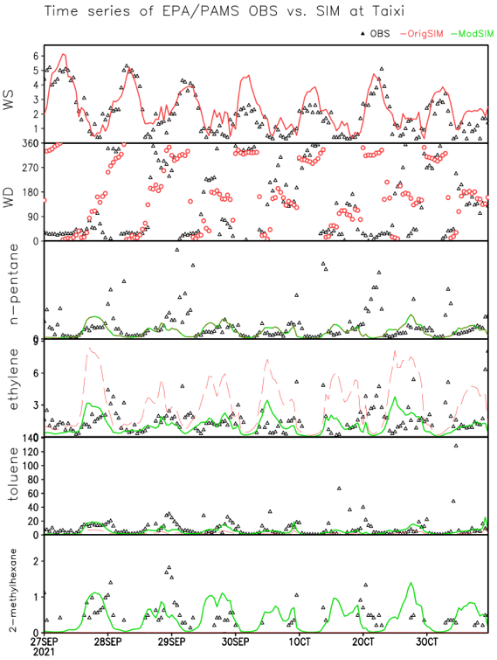
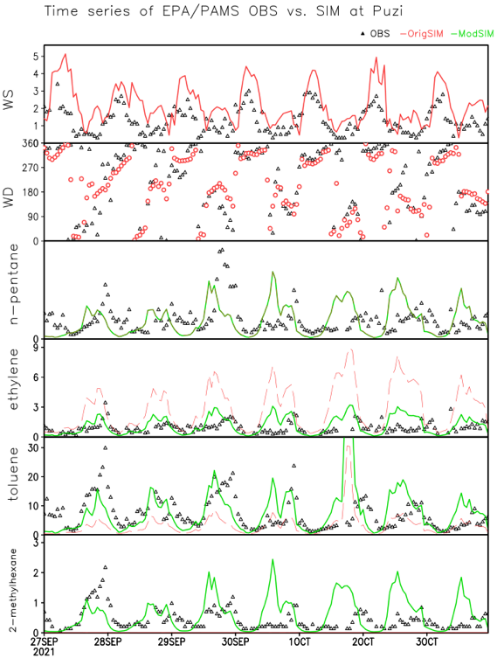


Fig. S3. Time series of observed and modeled wind fields and critical pollutants at PAMS stations for the 2021 case study.


Time series of EPA/PAMS OBS vs. SIM at Wanhua
▲ OBS —OrigSIM —ModSIM
WS
WD
n−pentane
ethylene
toluene
2−methylhexane
27SEP 2021
28SEP
29SEP
30SEP
1OCT
2OCT
3OCT


Time series of EPA/PAMS OBS vs. SIM at Tucheng
▲ OBS —OrigSIM —ModSIM
WS
WD
n−pentane
ethylene
toluene
2−methylhexane
27SEP 2021
28SEP
29SEP
30SEP
1OCT
2OCT
3OCT


Time series of EPA/PAMS OBS vs. SIM at Taixi
▲ OBS —OrigSIM —ModSIM
WS
WD
n−pentane
ethylene
toluene
2−methylhexane
27SEP 2021
28SEP
29SEP
30SEP
1OCT
2OCT
3OCT


Time series of EPA/PAMS OBS vs. SIM at Puzi
▲ OBS —OrigSIM —ModSIM
WS
WD
n−pentane
ethylene
toluene
2−methylhexane
27SEP 2021
28SEP
29SEP
30SEP
1OCT
2OCT
3OCT

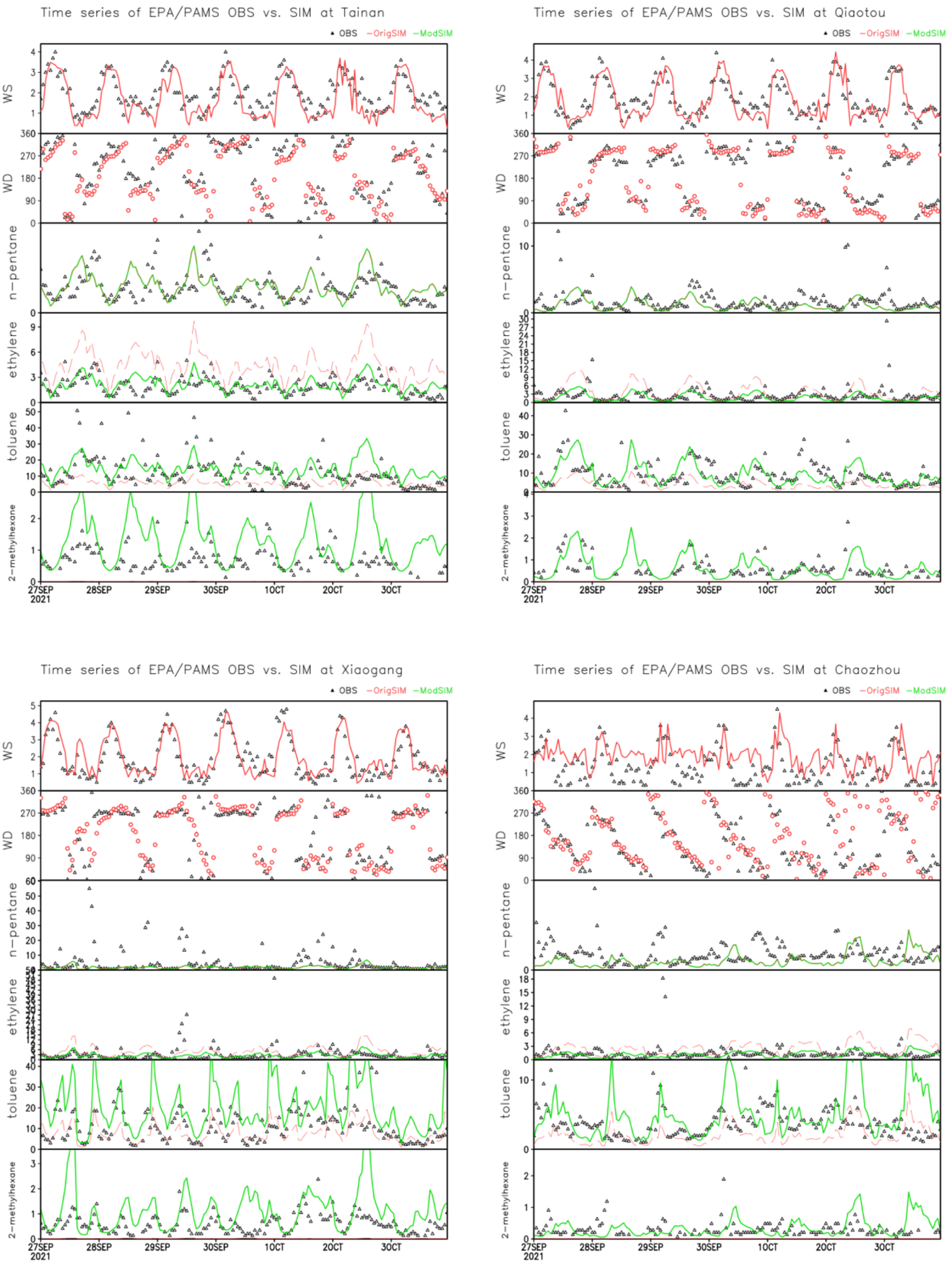


Fig. S4. All other PAMS sites exhibited similar results for PAMS species simulations (TPAMS, similar, underestimated, and overestimated patterns, as well as zero emissions).

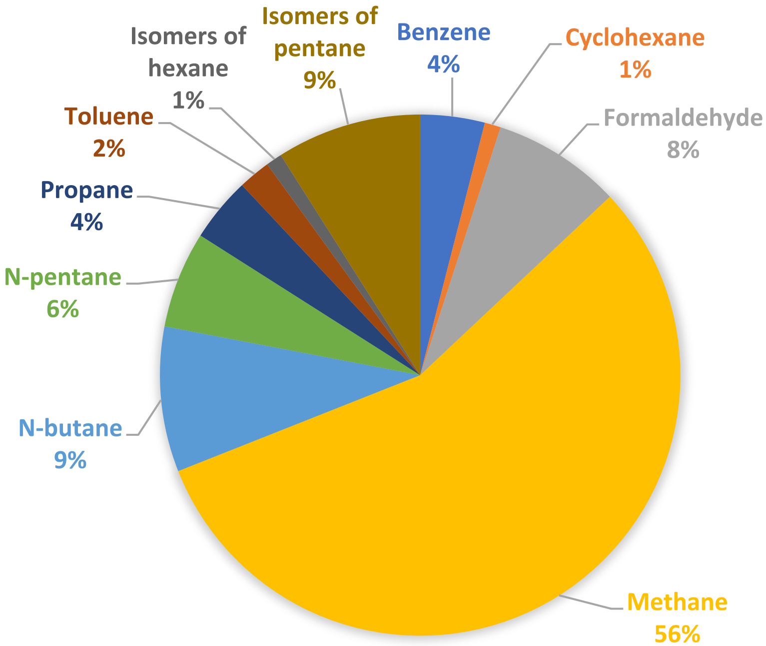


Fig. S5. VOC speciation profile for External Combustion Boiler – Natural Gas (0003).

Table S1. Mapping of 54 PAMS VOC species to their corresponding lumped surrogate species in the CB05e51 and CB6r3 chemical mechanisms.

PAMS Species Name	CB05e51	CB6r3
Acetylene	PAR	ETHY
Propane	PAR	PRPA
Isobutane	PAR	PAR
n-Butane	PAR	PAR
2,2-Dimethylbutane	PAR	PAR
Isopentane	PAR	PAR
n-Pentane	PAR	PAR
Cyclopentane	PAR	PAR
2,3-Dimethylbutane	PAR	PAR
2-Methylpentane	PAR	PAR
3-Methylpentane	PAR	PAR
n-Hexane	PAR	PAR
2,2,4-Trimethylpentane	PAR	PAR
Methylcyclopentane	PAR	PAR
2,4-Dimethylpentane	PAR	PAR
Cyclohexane	PAR	PAR
2-Methylhexane	PAR	PAR
2,3-Dimethylpentane	PAR	PAR
3-Methylhexane	PAR	PAR
n-Heptane	PAR	PAR
Methylcyclohexane	PAR	PAR
2,3,4-Trimethylpentane	PAR	PAR
2-Methylheptane	PAR	PAR
3-Methylheptane	PAR	PAR
n-Octane	PAR	PAR
n-Nonane	PAR	PAR
n-Decane	PAR	PAR
n-Undecane	PAR	PAR
trans-2-Butene	OLE	OLE
cis-2-Butene	OLE	OLE
trans-2-Pentene	OLE	OLE
cis-2-Pentene	OLE	OLE
Propylene	OLE	OLE
1-Butene	OLE	OLE
1-Pentene	OLE	OLE
Toluene	TOL	TOL
Ethylbenzene	BENZENE	BENZENE
Styrene	BENZENE	BENZENE
Isopropylbenzene	BENZENE	BENZENE
n-Propylbenzene	BENZENE	BENZENE
m,p-Xylene	XYLMN	XYLMN
o-Xylene	XYLMN	XYLMN
m-Ethyltoluene	XYLMN	XYLMN
p-Ethyltoluene	XYLMN	XYLMN

1,3,5-Trimethylbenzene	XYLMN	XYLMN
2-Ethyltoluene	XYLMN	XYLMN
1,2,4-Trimethylbenzene	XYLMN	XYLMN
1,2,3-Trimethylbenzene	XYLMN	XYLMN
m-Diethylbenzene	XYLMN	XYLMN
p-Diethylbenzene	XYLMN	XYLMN
Benzene	BENZENE	BENZENE
Ethane	ETHA	ETHA
Ethene	ETH	ETH
Isoprene	ISOP	ISOP

Table S2. Additional reaction pathways for PAMS species used in CMAQ-PAMS (CB6).

Species	ShortName	Reaction	Rate Expression*
Isobutane	iso-C4H10	iso-C4H10 + OH → XPAR	2.14E-12(T/298)^{2}e$^{213./T}$
n-Butane	n-C4H10	n-C4H10 + OH → XPAR	2.38E-12(T/298)^{2}e$^{114./T}$
2,2-Dimethylbutane	2,2-DMBa	2,2-DMBa + OH → XPAR	3.37E-11e$^{-809./T}$
Isopentane	iso-C5H12	iso-C5H12 + OH → XPAR	3.60E-12
n-Pentane	n-C5H12	n-C5H12 + OH → XPAR	3.84E-12(T/298)^{2}e$^{158./T}$
Cyclopentane	CPa	CPa + OH → XPAR	4.89E-12(T/298)^{2}e$^{214./T}$
2,3-Dimethylbutane	2,3-DMBa	2,3-DMBa + OH → XPAR	5.80E-12(T/298)^{2}e$^{407./T}$
2-Methylpentane	2-MPa	2-MPa + OH → XPAR	5.20E-12
3-Methylpentane	3-MPa	3-MPa + OH → XPAR	5.20E-12
n-Hexane	n-C6H14	n-C6H14 + OH → XPAR	5.25E-12(T/298)^{1}e$^{-112./T}$
2,2,4-Trimethylpentane	2,2,4-TMPa	2,2,4-TMPa + OH → XPAR	3.37E-12(T/298)^{2}e$^{140./T}$
Methylcyclopentane	MCPa	MCPa + OH → XPAR	8.60E-12
2,4-Dimethylpentane	2,4-DMPa	2,4-DMPa + OH → XPAR	2.49E-11e$^{-443./T}$
Cyclohexane	CHa	CHa + OH → XPAR	7.03E-12(T/298)^{2}e$^{262./T}$
2-Methylhexane	2-MHa	2-MHa + OH → XPAR	3.64E-11e$^{-380./T}$
2,3-Dimethylpentane	2,3-DMPa	2,3-DMPa + OH → XPAR	3.64E-11e$^{-380./T}$
3-Methylhexane	3-MHa	3-MHa + OH → XPAR	3.64E-11e$^{-380./T}$
n-Heptane	n-C7H16	n-C7H16 + OH → XPAR	6.79E-12(T/298)^{2}e$^{407./T}$
Methylcyclohexane	MCHa	MCHa + OH → XPAR	1.07E-11(T/298)^{2}e$^{342./T}$
2,3,4-Trimethylpentane	2,3,4-TMPa	2,3,4-TMPa + OH → XPAR	7.87E-12
2-Methylheptane	2-MHpa	2-MHpa + OH → XPAR	8.48E-12(T/298)^{2}e$^{354./T}$
3-Methylheptane	3-MHpa	3-MHpa + OH → XPAR	7.87E-12
n-Octane	n-C8H18	n-C8H18 + OH → XPAR	8.15E-12(T/298)^{2}e$^{361./T}$
n-Nonane	n-C9H20	n-C9H20 + OH → XPAR	9.74E-12(T/298)^{2}e$^{437./T}$
n-Decane	n-C10H22	n-C10H22 + OH → XPAR	1.10E-11(T/298)^{2}e$^{407./T}$
n-Undecane	n-C11H24	n-C11H24 + OH → XPAR	1.23E-11
trans-2-Butene	t-2-C4H8	t-2-C4H8 + O → 0.2000*ALD2 + 0.3000*ALDX + 0.1000*HO2 + 0.2000*XO2H + 0.2000*CO + 0.2000*FORM + 0.0100*XO2N + 0.2100*RO2 + 0.2000*PAR + 0.1000*OH	2.33E-11e$^{10./T}$
		t-2-C4H8 + OH → 0.7810*FORM + 0.4880*ALD2 + 0.4880*ALDX + 0.9760*XO2H + 0.1950*XO2 + 0.0240*XO2N + 1.1950*RO2 - 0.7300*PAR	1.01E-11e$^{548./T}$
		t-2-C4H8 + O3 → 0.2950*ALD2 + 0.5550*FORM + 0.2700*ALDX + 0.1500*XO2H + 0.1500*RO2 + 0.3340*OH + 0.0800*HO2 + 0.3780*CO + 0.0750*GLY + 0.0750*MGLY + 0.0900*FACD + 0.1300*AACD + 0.0400*H2O2 - 0.7900*PAR	5.90E-15e$^{1070./T}$
		t-2-C4H8 + NO3 → 0.5000*NO2 + 0.5000*NTR1 + 0.4800*XO2 + 0.4800*XO2H + 0.0400*XO2N + RO2 + 0.5000*FORM + 0.2500*ALD2 +	3.93E-13(T/298)^{2}e$^{382./T}$

		0.3750*ALDX - PAR	
cis-2-Butene	c-2-C4H8	c-2-C4H8 + O → 0.2000*ALD2 + 0.3000*ALDX + 0.1000*HO2 + 0.2000*XO2H + 0.2000*CO + 0.2000*FORM + 0.0100*XO2N + 0.2100*RO2 + 0.2000*PAR + 0.1000*OH	$1.79E-11e^{118./T}$
		c-2-C4H8 + OH → 0.7810*FORM + 0.4880*ALD2 + 0.4880*ALDX + 0.9760*XO2H + 0.1950*XO2 + 0.0240*XO2N + 1.1950*RO2 - 0.7300*PAR	$1.22E-11e^{546./T}$
		c-2-C4H8 + O3 → 0.2950*ALD2 + 0.5550*FORM + 0.2700*ALDX + 0.1500*XO2H + 0.1500*RO2 + 0.3340*OH + 0.0800*HO2 + 0.3780*CO + 0.0750*GLY + 0.0750*MGLY + 0.0900*FACD + 0.1300*AACD + 0.0400*H2O2 - 0.7900*PAR	$5.59E-15e^{1020./T}$
		c-2-C4H8 + NO3 → 0.5000*NO2 + 0.5000*NTR1 + 0.4800*XO2 + 0.4800*XO2H + 0.0400*XO2N + RO2 + 0.5000*FORM + 0.2500*ALD2 + 0.3750*ALDX - PAR	$3.93E-13(T/298)^{2}e^{382./T}$
trans-2-Pentene	t-2-C5H10	t-2-C5H10 + O → 0.2000*ALD2 + 0.3000*ALDX + 0.1000*HO2 + 0.2000*XO2H + 0.2000*CO + 0.2000*FORM + 0.0100*XO2N + 0.2100*RO2 + 0.2000*PAR + 0.1000*OH	$2.24E-11(T/298)^{1.14}$
		t-2-C5H10 + OH → 0.7810*FORM + 0.4880*ALD2 + 0.4880*ALDX + 0.9760*XO2H + 0.1950*XO2 + 0.0240*XO2N + 1.1950*RO2 - 0.7300*PAR	$1.11E-11e^{566./T}$
		t-2-C5H10 + O3 → 0.2950*ALD2 + 0.5550*FORM + 0.2700*ALDX + 0.1500*XO2H + 0.1500*RO2 + 0.3340*OH + 0.0800*HO2 + 0.3780*CO + 0.0750*GLY + 0.0750*MGLY + 0.0900*FACD + 0.1300*AACD + 0.0400*H2O2 - 0.7900*PAR	$5.90E-15e^{1070./T}$
		t-2-C5H10 + NO3 → 0.5000*NO2 + 0.5000*NTR1 + 0.4800*XO2 + 0.4800*XO2H + 0.0400*XO2N + RO2 + 0.5000*FORM + 0.2500*ALD2 + 0.3750*ALDX - PAR	$3.93E-13(T/298)^{2}e^{382./T}$
cis-2-Pentene	c-2-C5H10	c-2-C5H10 + O → 0.2000*ALD2 + 0.3000*ALDX + 0.1000*HO2 + 0.2000*XO2H + 0.2000*CO + 0.2000*FORM + 0.0100*XO2N + 0.2100*RO2 + 0.2000*PAR + 0.1000*OH	$1.63E-11(T/298)^{1.12}$
		c-2-C5H10 + OH → 0.7810*FORM + 0.4880*ALD2 + 0.4880*ALDX +	$1.56E-11e^{532./T}$

		0.9760*XO2H + 0.1950*XO2 + 0.0240*XO2N + 1.1950*RO2 - 0.7300*PAR	
		c-2-C5H10 + O3 → 0.2950*ALD2 + 0.5550*FORM + 0.2700*ALDX + 0.1500*XO2H + 0.1500*RO2 + 0.3340*OH + 0.0800*HO2 + 0.3780*CO + 0.0750*GLY + 0.0750*MGLY + 0.0900*FACD + 0.1300*AACD + 0.0400*H2O2 - 0.7900*PAR	$5.59E-15e^{1020./T}$
		c-2-C5H10 + NO3 → 0.5000*NO2 + 0.5000*NTR1 + 0.4800*XO2 + 0.4800*XO2H + 0.0400*XO2N + RO2 + 0.5000*FORM + 0.2500*ALD2 + 0.3750*ALDX - PAR	$3.93E-13(T/298)^{2}e^{382./T}$
Propylene	C3H6	C3H6 + O → 0.2000*ALD2 + 0.3000*ALDX + 0.1000*HO2 + 0.2000*XO2H + 0.2000*CO + 0.2000*FORM + 0.0100*XO2N + 0.2100*RO2 + 0.2000*PAR + 0.1000*OH	$4.43E-12e^{-259./T}$
		C3H6 + OH → 0.7810*FORM + 0.4880*ALD2 + 0.4880*ALDX + 0.9760*XO2H + 0.1950*XO2 + 0.0240*XO2N + 1.1950*RO2 - 0.7300*PAR	$4.85E-12e^{504./T}$
		C3H6 + O3 → 0.2950*ALD2 + 0.5550*FORM + 0.2700*ALDX + 0.1500*XO2H + 0.1500*RO2 + 0.3340*OH + 0.0800*HO2 + 0.3780*CO + 0.0750*GLY + 0.0750*MGLY + 0.0900*FACD + 0.1300*AACD + 0.0400*H2O2 - 0.7900*PAR	$5.50E-15e^{-1880./T}$
		C3H6 + NO3 → 0.5000*NO2 + 0.5000*NTR1 + 0.4800*XO2 + 0.4800*XO2H + 0.0400*XO2N + RO2 + 0.5000*FORM + 0.2500*ALD2 + 0.3750*ALDX - PAR	$6.79E-13e^{-2160./T}$
1-Butene	1-C4H8	1-C4H8 + O → 0.2000*ALD2 + 0.3000*ALDX + 0.1000*HO2 + 0.2000*XO2H + 0.2000*CO + 0.2000*FORM + 0.0100*XO2N + 0.2100*RO2 + 0.2000*PAR + 0.1000*OH	$4.56E-12e^{-336./T}$
		1-C4H8 + OH → 0.7810*FORM + 0.4880*ALD2 + 0.4880*ALDX + 0.9760*XO2H + 0.1950*XO2 + 0.0240*XO2N + 1.1950*RO2 - 0.7300*PAR	$6.54E-12e^{468./T}$
		1-C4H8 + O3 → 0.2950*ALD2 + 0.5550*FORM + 0.2700*ALDX + 0.1500*XO2H + 0.1500*RO2 + 0.3340*OH + 0.0800*HO2 + 0.3780*CO + 0.0750*GLY + 0.0750*MGLY + 0.0900*FACD + 0.1300*AACD + 0.0400*H2O2 - 0.7900*PAR	$3.40E-15e^{-1800./T}$

		1-C4H8 + NO3 → 0.5000*NO2 + 0.5000*NTR1 + 0.4800*XO2 + 0.4800*XO2H + 0.0400*XO2N + RO2 + 0.5000*FORM + 0.2500*ALD2 + 0.3750*ALDX - PAR	$1.40E-12e^{-1460./T}$
1-Pentene	1-C5H10	1-C5H10 + O → 0.2000*ALD2 + 0.3000*ALDX + 0.1000*HO2 + 0.2000*XO2H + 0.2000*CO + 0.2000*FORM + 0.0100*XO2N + 0.2100*RO2 + 0.2000*PAR + 0.1000*OH	$1.66E-11e^{13./T}$
		1-C5H10 + OH → 0.7810*FORM + 0.4880*ALD2 + 0.4880*ALDX + 0.9760*XO2H + 0.1950*XO2 + 0.0240*XO2N + 1.1950*RO2 - 0.7300*PAR	3.12E-11
		1-C5H10 + O3 → 0.2950*ALD2 + 0.5550*FORM + 0.2700*ALDX + 0.1500*XO2H + 0.1500*RO2 + 0.3340*OH + 0.0800*HO2 + 0.3780*CO + 0.0750*GLY + 0.0750*MGLY + 0.0900*FACD + 0.1300*AACD + 0.0400*H2O2 - 0.7900*PAR	$7.60E-15e^{-1977./T}$
		1-C5H10 + NO3 → 0.5000*NO2 + 0.5000*NTR1 + 0.4800*XO2 + 0.4800*XO2H + 0.0400*XO2N + RO2 + 0.5000*FORM + 0.2500*ALD2 + 0.3750*ALDX - PAR	$2.60E-11e^{-1699./T}$
Toluene	TOL	TOL + OH → 0.1800*CRES + 0.6500*TO2 + 0.7200*RO2 + 0.1000*OPEN + 0.1000*OH + 0.0700*XO2H + 0.1800*HO2 + TOLRO2	$1.81E-11e^{360./T}$
Ethylbenzene	EB	EB + OH → 0.5300*CRES + 0.3520*BZO2 + 0.3520*RO2 + 0.1180*OPEN + 0.1180*OH + 0.5300*HO2 + BENZRO2	$7.00E-12e^{340./T}$
Styrene	STY	STY + OH → 0.5300*CRES + 0.3520*BZO2 + 0.3520*RO2 + 0.1180*OPEN + 0.1180*OH + 0.5300*HO2 + BENZRO2	5.86E-11
Isopropylbenzene	iso-PB	iso-PB + OH → 0.5300*CRES + 0.3520*BZO2 + 0.3520*RO2 + 0.1180*OPEN + 0.1180*OH + 0.5300*HO2 + BENZRO2	6.61E-12
n-Propylbenzene	n-PB	n-PB + OH → 0.5300*CRES + 0.3520*BZO2 + 0.3520*RO2 + 0.1180*OPEN + 0.1180*OH + 0.5300*HO2 + BENZRO2	5.71E-12
m,p-Xylenes	m,p-XYL	m,p-XYL + OH → 0.155*CRES + 0.544*XLO2 + 0.602*RO2 + 0.244*XOPN + 0.244*OH + 0.058*XO2H + 0.155*HO2 + XYLRO2	$1.66E-11e^{115./T}$
o-Xylene	o-XYL	o-XYL + OH → 0.155*CRES + 0.544*XLO2 + 0.602*RO2 + 0.244*XOPN + 0.244*OH + 0.058*XO2H + 0.155*HO2 + XYLRO2	1.47E-11

m-Ethyltoluene	m-ETol	m-ETol + OH → 0.155*CRES + 0.544*XLO2 + 0.602*RO2 + 0.244*XOPN + 0.244*OH + 0.058*XO2H + 0.155*HO2 + XYLRO2	2.24E-11
p-Ethyltoluene	p-ETol	p-ETol + OH → 0.155*CRES + 0.544*XLO2 + 0.602*RO2 + 0.244*XOPN + 0.244*OH + 0.058*XO2H + 0.155*HO2 + XYLRO2	1.36E-11
1,3,5-Trimethylbenzene	1,3,5-TMB	1,3,5-TMB + OH → 0.155*CRES + 0.544*XLO2 + 0.602*RO2 + 0.244*XOPN + 0.244*OH + 0.058*XO2H + 0.155*HO2 + XYLRO2	5.75E-11
o-Ethyltoluene	o-ETol	o-ETol + OH → 0.155*CRES + 0.544*XLO2 + 0.602*RO2 + 0.244*XOPN + 0.244*OH + 0.058*XO2H + 0.155*HO2 + XYLRO2	1.32E-11
1,2,4-Trimethylbenzene	1,2,4-TMB	1,2,4-TMB + OH → 0.155*CRES + 0.544*XLO2 + 0.602*RO2 + 0.244*XOPN + 0.244*OH + 0.058*XO2H + 0.155*HO2 + XYLRO2	3.25E-11
1,2,3-Trimethylbenzene	1,2,3-TMB	1,2,3-TMB + OH → 0.155*CRES + 0.544*XLO2 + 0.602*RO2 + 0.244*XOPN + 0.244*OH + 0.058*XO2H + 0.155*HO2 + XYLRO2	3.32E-11
m-Diethylbenzene	m-DEB	m-DEB + OH → 0.155*CRES + 0.544*XLO2 + 0.602*RO2 + 0.244*XOPN + 0.244*OH + 0.058*XO2H + 0.155*HO2 + XYLRO2	1.89E-11e$^{116./T}$
p-Diethylbenzene	p-DEB	p-DEB + OH → 0.155*CRES + 0.544*XLO2 + 0.602*RO2 + 0.244*XOPN + 0.244*OH + 0.058*XO2H + 0.155*HO2 + XYLRO2	1.89E-11e$^{116./T}$

*** Units for rate constants of reactions are cm^3 molecule^{-1} s^{-1}.**

Table S3. Proportional contributions of PAMS species within each CB6 lumped VOC group, based on domain-wide anthropogenic emissions (unit: moles s^{-1}).

PAMS species	CB6 lump species	Domain total emission (moles/s)	Mass fraction
Acetylene	ETHY	2.95	1.00
Propane	PRPA	2.54	1.00
Isobutane	PAR	1.77	0.06
n-Butane	PAR	9.81	0.35
2,2-Dimethylbutane	PAR	0.12	0.00
Isopentane	PAR	4.61	0.16
n-Pentane	PAR	2.39	0.09
Cyclopentane	PAR	0.26	0.01
2,3-Dimethylbutane	PAR	0.40	0.01
2-Methylpentane	PAR	1.05	0.04
3-Methylpentane	PAR	0.65	0.02
n-Hexane	PAR	0.98	0.03
2,2,4-Trimethylpentane	PAR	0.83	0.03
Methylcyclopentane	PAR	0.55	0.02
2,4-Dimethylpentane	PAR	0.29	0.01
Cyclohexane	PAR	1.31	0.05
2-Methylhexane	PAR	0.01	0.00
2,3-Dimethylpentane	PAR	0.63	0.02
3-Methylhexane	PAR	0.48	0.02
n-Heptane	PAR	0.71	0.03
Methylcyclohexane	PAR	0.29	0.01
2,3,4-Trimethylpentane	PAR	0.06	0.00
2-Methylheptane	PAR	0.08	0.00
3-Methylheptane	PAR	0.15	0.01
n-Octane	PAR	0.19	0.01
n-Nonane	PAR	0.09	0.00
n-Decane	PAR	0.15	0.01
n-Undecane	PAR	0.20	0.01
trans-2-Butene	OLE	0.50	0.09
cis-2-Butene	OLE	0.44	0.08
trans-2-Pentene	OLE	0.47	0.09
cis-2-Pentene	OLE	0.28	0.05
Propylene	OLE	2.52	0.45
1-Butene	OLE	0.94	0.17
1-Pentene	OLE	0.41	0.07
Toluene	TOL	4.53	1.00
Ethylbenzene	BENZENE	0.57	0.12
Styrene	BENZENE	1.78	0.38
Isopropylbenzene	BENZENE	0.08	0.02
n-Propylbenzene	BENZENE	0.20	0.04
Benzene	BENZENE	2.01	0.43
m,p-Xylenes	XYLMN	1.46	0.28
o-Xylene	XYLMN	0.90	0.17
m-Ethyltoluene	XYLMN	0.41	0.08

p-Ethyltoluene	XYLMN	0.00	0.00
1,3,5-Trimethylbenzene	XYLMN	0.98	0.19
o-Ethyltoluene	XYLMN	0.01	0.00
1,2,4-Trimethylbenzene	XYLMN	0.98	0.19
1,2,3-Trimethylbenzene	XYLMN	0.25	0.05
m-Diethylbenzene	XYLMN	0.20	0.04
p-Diethylbenzene	XYLMN	0.00	0.00
Ethane	ETHA	3.75	1.00
Ethene (Ethylene)	ETH	20.21	1.00

Note: Isoprene (PAMS56) is not included in Table S3 because it is treated as a biogenic VOC in the emission inventory. As the purpose of Table S3 is to document anthropogenic VOC speciation and its mapping to CB6 lumped groups, biogenic species are excluded.

Table S4. Comparison of model simulations with observations at all general TAQMN sites in Taiwan*.

	WS	NO_x	VOCs	O_3
Mean observed value	1.86	11.85	99.96	38.65
Mean modeled value	2.29	10.93	151.94	32.69
MB	0.43	-0.84	53.41	-5.86
RMSE	1.33	12.36	122.12	16.52
R	0.62	0.33	0.33	0.70
R^2	0.39	0.11	0.11	0.49
NMB(%)	23.20	-7.07	53.43	-15.15
NME(%)	51.08	60.92	92.10	33.11

	WD
Mean observed value	164.16
Mean modeled value	165.35
WNMB	-0.76
WNME	13.24

*Model period is from September 27, 2021 to October 3, 2021. Definitions of model evaluation metrics can be referred to as in Chen et al. (2021).

Table S5. Averages of PAMS VOC observations and simulations.

Group	Species	ModSIM	OBS
Alkanes	propane	4.33	4.51
	isobutane	2.98	2.83
	n-butane	3.91	3.95
	2,2-dimethylbutane	0.27	0.20
	isopentane	4.15	4.08
	n-pentane	1.40	1.74
	2,3-dimethylbutane	0.37	0.33
	2-methylpentane	1.06	0.86
	3-methylpentane	0.91	0.81
	n-hexane	1.50	1.40
	2,2,4-trimethylpentane	0.73	0.97
	2,4-dimethylpentane	0.47	0.39
	2-methylhexane	0.94	0.8
	2,3-dimethylpentane	0.57	0.46
	3-methylhexane	0.37	0.89
	n-heptane	0.86	0.66
	2,3,4-trimethylpentane	0.03	0.41
	2-methylheptane	0.29	0.24
	3-methylheptane	0.39	0.24
	n-octane	0.35	0.36
	n-nonane	0.33	0.38
	n-decane	0.31	0.45
	n-undecane	0.32	0.36
	ethane	4.24	3.93
Cycloalkanes	cyclopentane	0.55	0.54
	methylcyclopentane	0.47	0.41
	cyclohexane	0.56	0.64
	methylcyclohexane	0.95	0.97
Alkenes	trans-2-butene	0.38	0.42
	cis-2-butene	0.25	0.29
	trans-2-pentene	0.27	0.29
	cis-2-pentene	0.13	0.17
	propylene	1.07	1.40
	1-butene	0.45	0.55
	1-pentene	0.15	0.22
	isoprene	2.56	1.54
	ethylene	2.06	1.95
Alkynes	acetylene	2.24	2.22
Aromatics	benzene	0.34	1.67
	toluene	12.73	11.43
	ethylbenzene	1.40	1.31
	styrene	0.46	0.60
	isopropylbenzene	0.21	0.27
	n-propylbenzene	0.39	0.36
	m,p-xylenes	4.34	3.75
	o-xylene	1.67	1.47
	m-ethyltoluene	1.00	0.88
	p-ethyltoluene	0.81	0.59
	o-ethyltoluene	0.71	0.44
	1,2,4-trimethylbenzene	1.75	1.53
	1,2,3-trimethylbenzene	0.73	0.69
	1,3,5-trimethylbenzene	0.53	0.48
	m-diethylbenzene	0.18	0.19
	p-diethylbenzene	0.35	0.38

The unit of OBS and SIM averages is ppbC.

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