Science Team Telecon (17/18 June 2024)

Agenda

- Data Archive Status and Time Synchronization of DC-8 data
- Changmin Cho – Ozone and Nitrate Formation Sensitivity
- Joo-Ae Kim – Ground Measurement of VOCs in Seoul
- Update from Thai Steering Group
- Brainstorming Updates
- Organizing the Roadmap Ahead

ASIA-AQ Preliminary Data Status

DC-8	Philippines	Philippines	Philippines	Philippines	Taiwan	Korea	Korea	Korea	Korea	Korea	Taiwan	Thailand	Thailand	Thailand	Thailand	Taiwan
	6-Feb	7-Feb	11-Feb	13-Feb	15-Feb	17-Feb	26-Feb	8-Mar	10-Mar	11-Mar	13-Mar	16-Mar	18-Mar	21-Mar	25-Mar	27-Mar
TOGA																
NSERC																
WAS																
TILDAS																
CIT-CIMS																
DACOM																
DLH																
NONO2O3																
MMS																
CAFS																
GTCIMS																
CU-AMS																
K-CIMS																
LGR-AAT																
K-SP2																
K-AMS																
K-SP2D																
K-SMPS																
Smoke Flag																
CAESAR																
LARGE																
LARGE-SP2																
MIRO																
ROZE																
CANOE																
PTR-MS																
CHARON																
ISAF																
K-CCN																
OPALS																
Profile Flag																

- submitted
- partial submission
- no data collected
- not submitted

New profile flag has been added to the archive! Please consult files in archive listed under “Silverman”

ASIA-AQ Preliminary Data Status

1900D	17-Feb	23-Feb	26-Feb	28-Feb	2-Mar	3-Mar	4-Mar	7-Mar	8-Mar	10-Mar
AIMMS										
CO-CH4-CO2										
O3										
NO2										
HCHO										
NH3										
AMS										
SP2										

C90 GT	17-Feb	23-Feb	26-Feb	1-Mar	3-Mar	4-Mar	8-Mar	9-Mar	10-Mar
AIMMS									
CO-CH4-CO2									
LGR-NH3									
TAP-BC									
NO2									
O3									
SO2									

350HW	7-Feb	17-Feb	23-Feb	26-Feb	7-Mar	8-Mar	9-Mar	11-Mar
AIMMS								
CO-CH4-CO2								

submitted
partial submission
no data collected
not submitted

G-III	Philippines	Philippines	Philippines	Philippines	Philippines	Taiwan	Korea	Korea	Korea	Korea	Korea	Korea	Korea	Korea	Korea	Taiwan	Thailand	Thailand	Thailand	Thailand	Thailand	Thailand	Taiwan
	6-Feb	7-Feb	10-Feb	11-Feb	13-Feb	15-Feb	17-Feb	23-Feb	26-Feb	28-Feb	1-Mar	2-Mar	3-Mar	8-Mar	10-Mar	13-Mar	16-Mar	18-Mar	19-Mar	21-Mar	23-Mar	25-Mar	27-Mar
HSRL2																							
GCAS																							

Time Synchronization of Final Data for DC-8

- As in previous campaigns, DC-8 investigators need to synchronize their final data.
- The DLH 1 Hz measurement serves as the reference time base. Even though it is preliminary, it has variability that is GPS synched.
- Please examine the variability of your measurements against DLH to determine your time shift and adjust your final data accordingly.
- Vertical profiles are often ideal for tracking differences in timing.
- Also checking individual plumes is recommended when performing analysis at 1 hz or faster.
- If you need final RH values for data processing, please reach out to Josh Digangi or Glenn Diskin.

Brainstorming (from last time)

- Korea: offshore pollution demonstrating what can be potentially transported. Origin, age, fire contribution?
- All: Demonstrate that missed approaches are a viable sampling strategy and show much greater variability than expected.
- Thailand: Examine the shift in GEMS HCHO. Is it real? Fires vs biogenics.
- All: Examine differences in constituent profile shapes and perturbation depths.
- Thailand: Examine similarities and differences in emission ratios for Thai smoke versus crop fires and wildfires during FIREX-AQ.
- Thailand: Examine relationship between O3 and HCHO in GEMS and Pandora observations
- All: Evaluate the effectiveness of the air quality monitoring network
- Philippines and Thailand: Examine the role of black carbon.
- Thailand: Characterize north-south gradients in aerosol composition…extent of fire influence
- Philippines: What's up with ozone? Why is it not higher over Manila.
- Philippines: How important is the sea salt contribution to PM2.5?
- Taiwan: Characterize VOC mixtures and toxics in Kaohsiung.
- All: Compare footprint of ascents and descents compared to spiral profiling (and duration and location)
- All: Evaluate whether the surface temperature measurement offers any insight into PBLH and urban heat island effects.

Brainstorming (continued)

- **Philippines: Assuming similar emission profiles on the different flight days, what are the conditions that lead to polluted days and relatively cleaner days (given the complex topography of Manila and the Northeast monsoon season)**
- **Philippines: How do conditions on the more polluted and cleaner days help to inform the aerosol-meteorology relationship.**

Organizing the Roadmap Ahead

Rough timeline and milestones:

1 October 2024 - Final Data Submission and Public Release

(develop questions and outlines for synthesis reports by this date)

20-24 January 2025 - Science Team Meeting - hosted by UKM in Malaysia

(5 days - one day dedicated to each country with talks, posters, and breakouts to further develop draft synthesis reports)

Mid-February to mid-March 2025 - Deliver and publicize synthesis reports in each country

Analyzing ozone and nitrate formation sensitivity in mega cities during ASIA-AQ

Changmin Cho, Alessandro Franchin, Courtney Owen, Kirk Lesko, and ASIA-AQ team

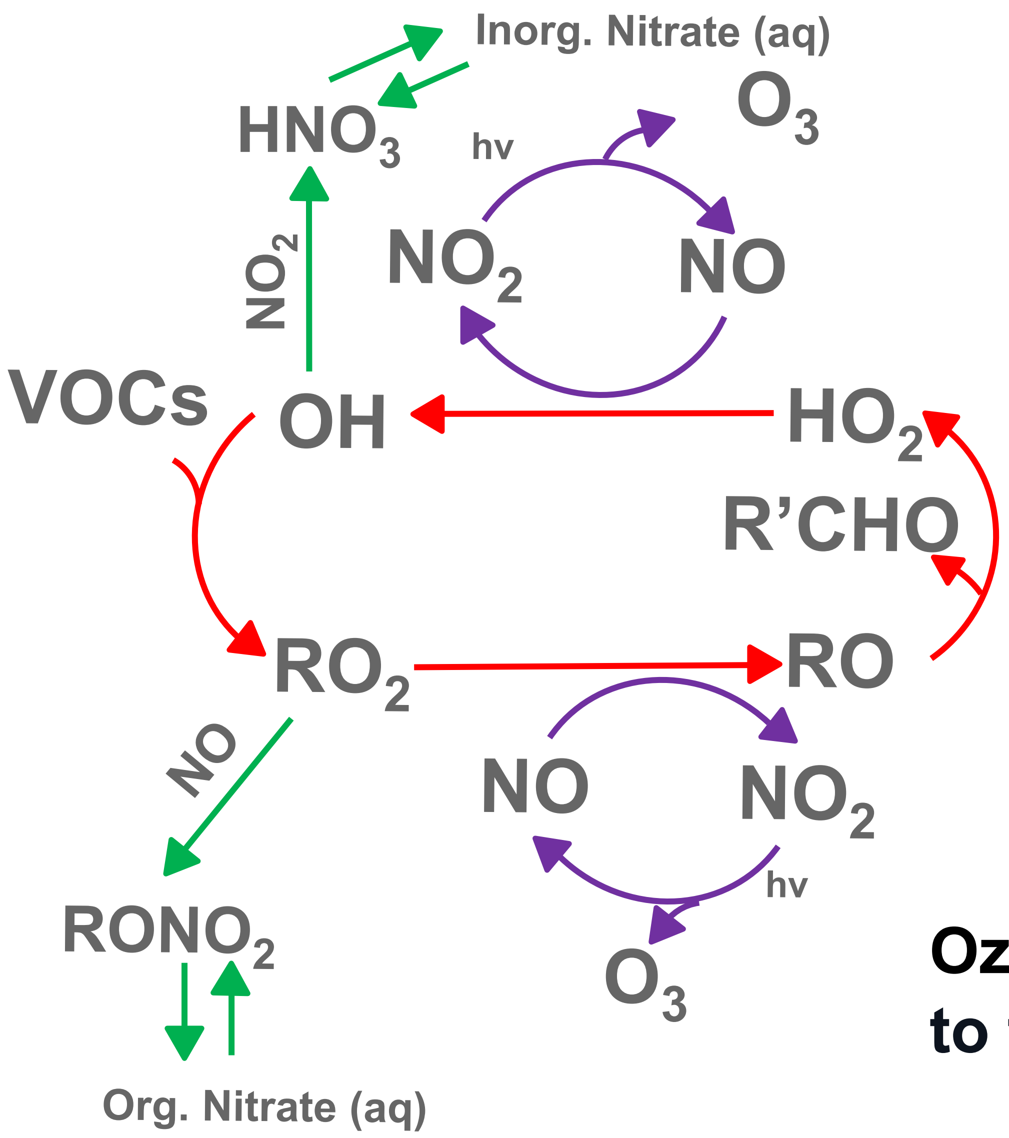
NOxO3 group, Atmospheric Chemistry Observations & Modeling (ACOM), National Center for Atmospheric Research (NCAR)

Contact: changminc@ucar.edu

June 13, 2024

This material is based upon work supported by the National Center for Atmospheric Research, which is a major facility sponsored by the National Science Foundation under Cooperative Agreement No. 1852977.

Ozone and Nitrate formation mechanism



O_X production rate

$$\mathrm{netP_{Ox}} = \mathrm{k_{NO+HO_2}[NO][HO_2] + k_{NO+RO_2}[NO][RO_2] - k_{OH+NO_2}[OH][NO_2]}$$

HNO_3 production rate

$$P_{\mathrm{HNO3}} = \mathrm{k_{OH+NO_2}[OH][NO_2]} \xrightarrow{\mathrm{NH_3}} \text{Inorg. Nitrate (aq)}$$

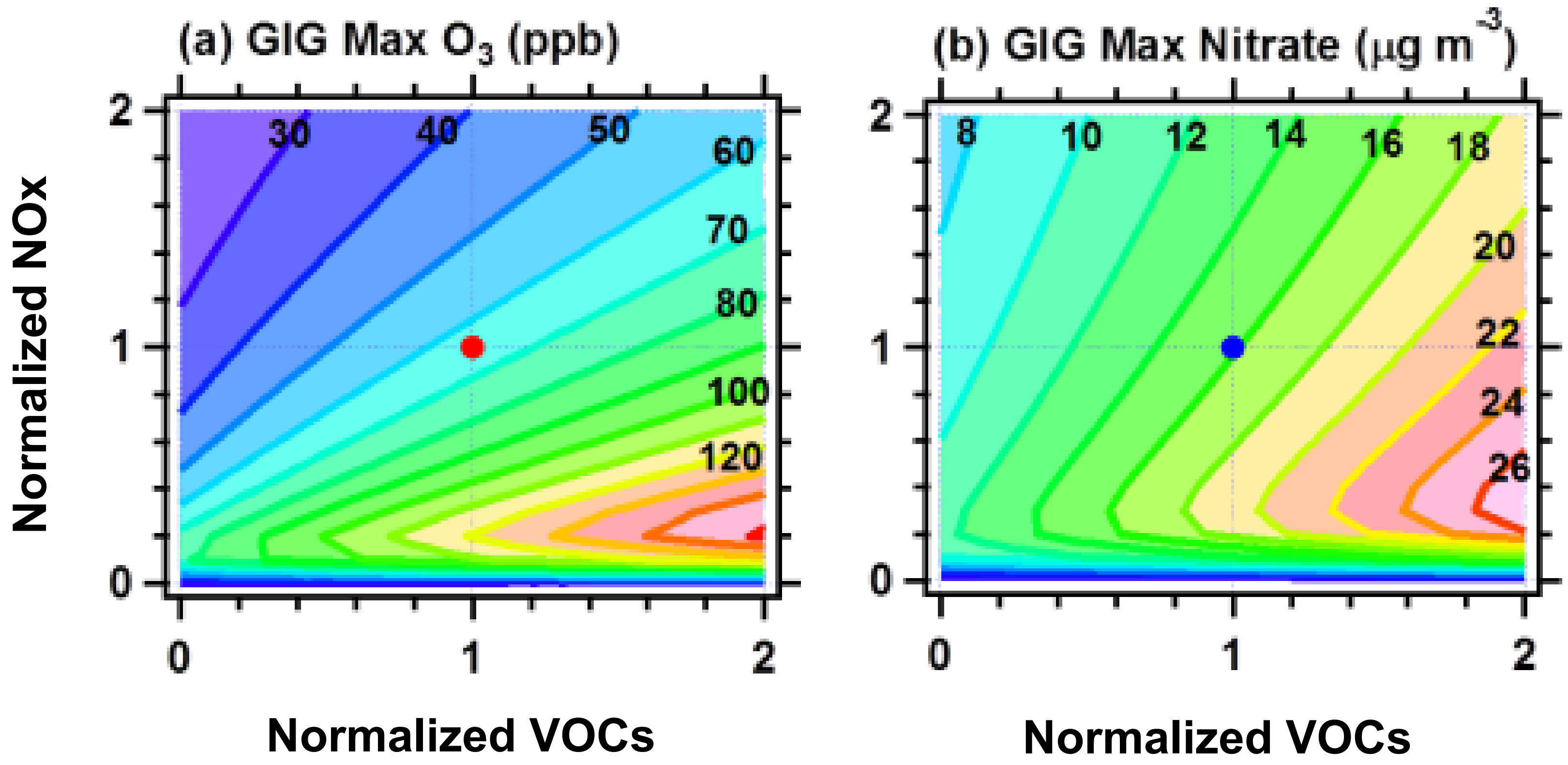
ANs production rate

$$P_{\mathrm{ANs}} = \alpha \mathrm{k_{RO_2+NO}[RO_2][NO]} \longrightarrow \text{Org. Nitrate (aq)}$$

(α: ANs branching ratio of RO_2+NO)

Ozone and Nitrate formation is highly non-linear to the changes of precursors

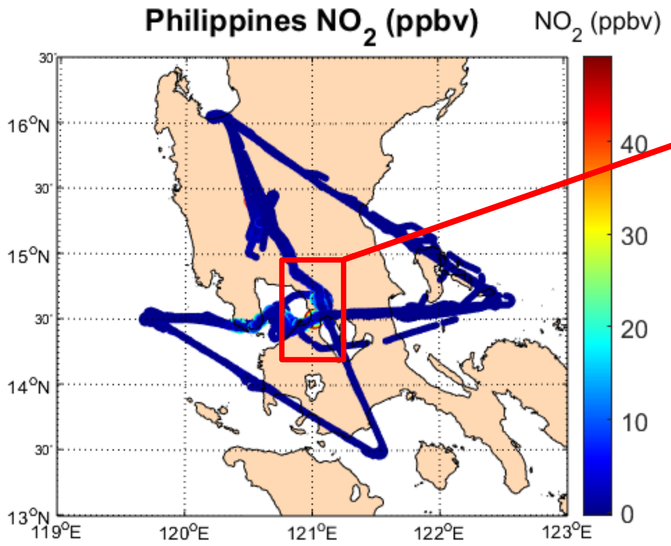
Ozone and Nitrate formation mechanism



It is important to understand where we are for Ozone & Nitrate pollution control!

Yang et al., ACP, 22, 4539–4556, 2022

ASIA-AQ DC-8 flights

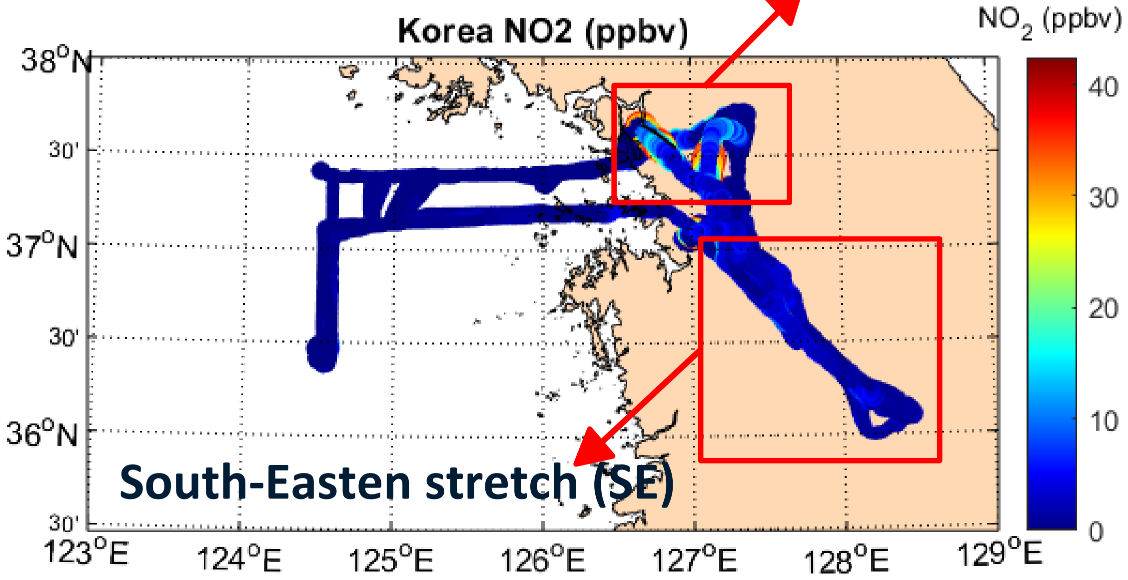


Metro Manila (MM)

Feb. 6, 7, 11, 13

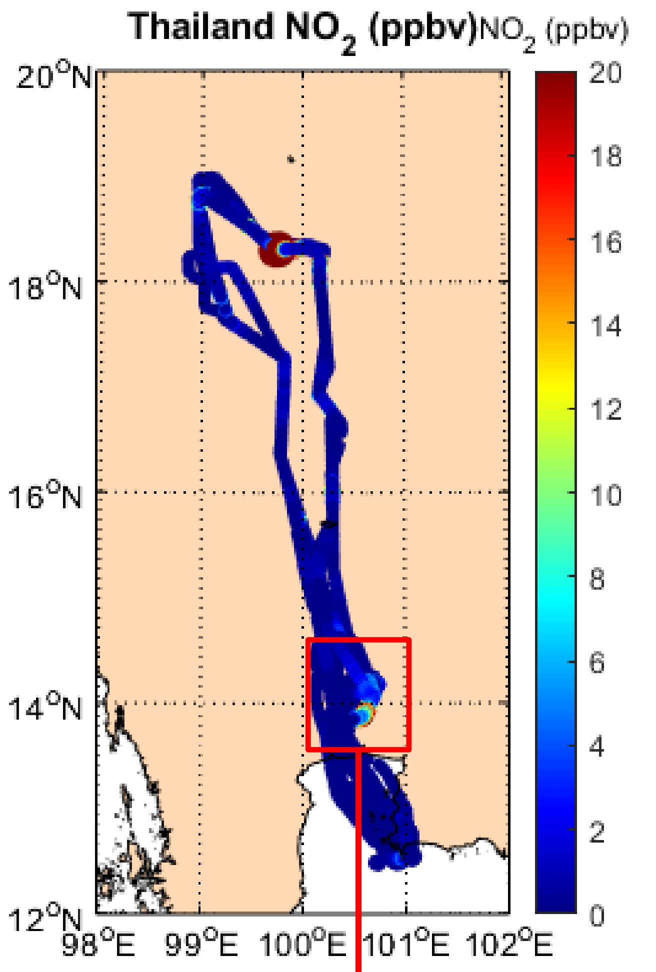
Feb. 17, 26 & Mar. 8, 10 ,11

Seoul Metropolitan Area (SMA)



South-Easten stretch (SE)

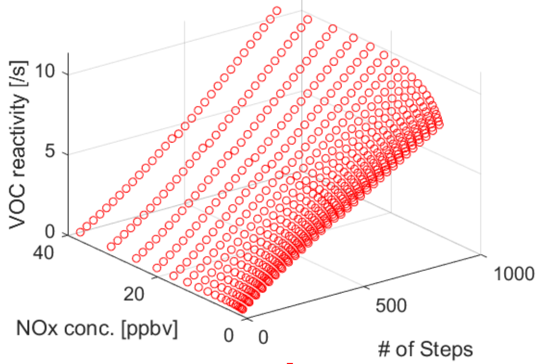
Mar. 16, 18, 21, 25



Bangkok Metropolitan Region (BMR)

Framework for 0-D Atmospheric Modeling (F0AM)

NOx Grid: 0-40ppbv
VOC Grid: 0-10/s

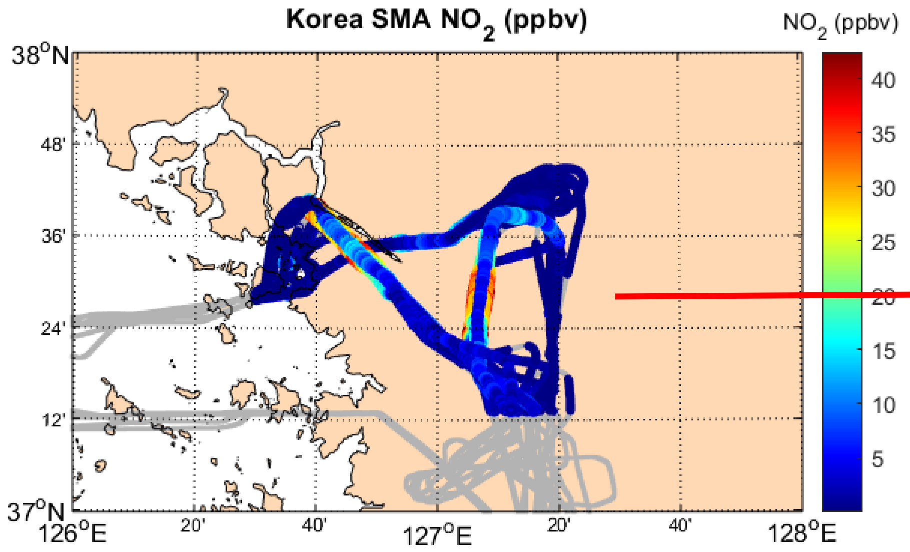


Constraints: P, T, H_2O, J-values, CO, CH_4, O_3, NO_x, HCHO, and VOCs from WAS and TOGA (filtered to be below 5000ft and mid-day (11:00-15:00))

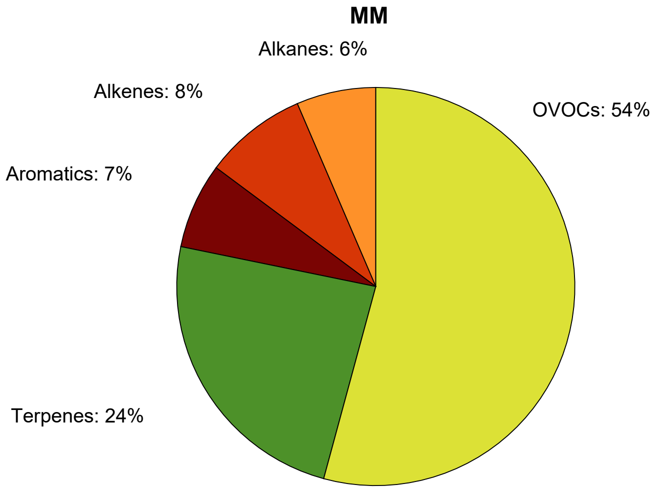
Mechanism: MCMv331

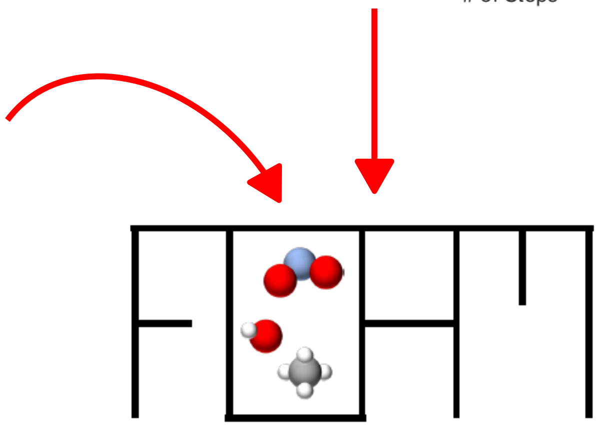
Dilution: 24-hour physical loss lifetime for all species

Using Solar cycle mode (3 days looping) for steady-state simulations along a flight transect



Observed VOC speciation

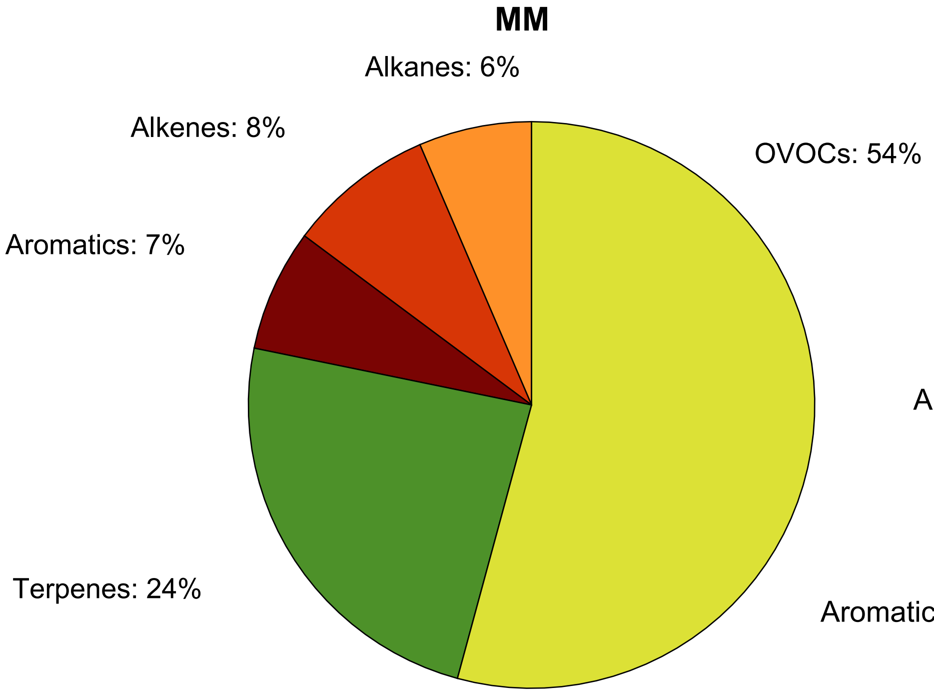




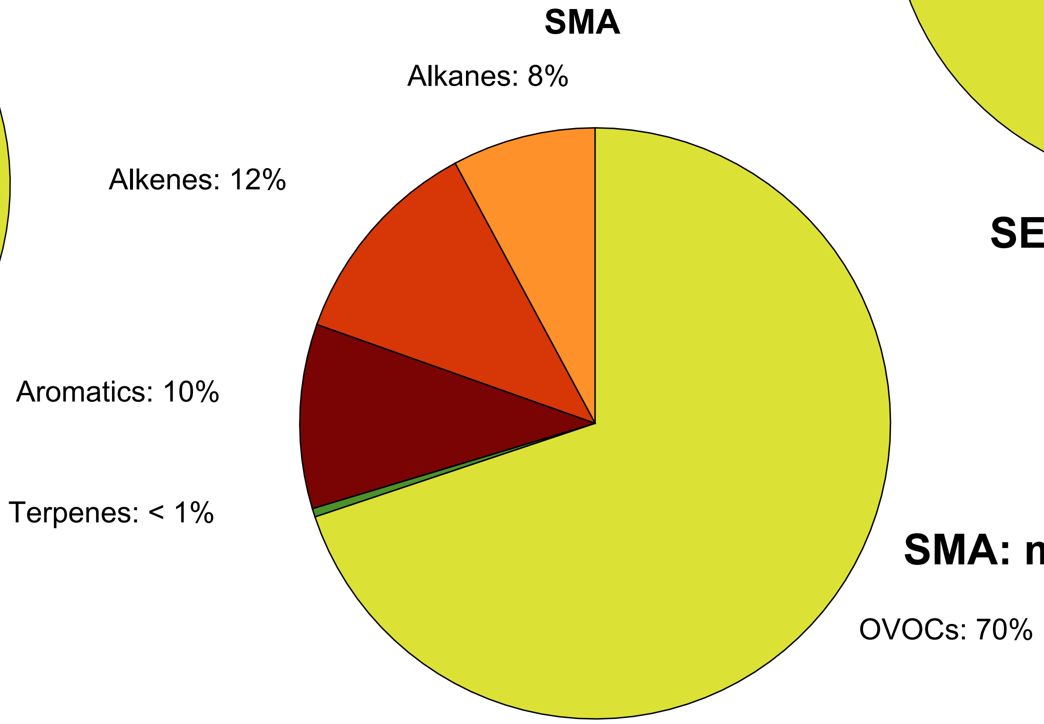
Wolfe et al., GMD, 9, 3309–3319, 2016

VOC Reactivity Speciation

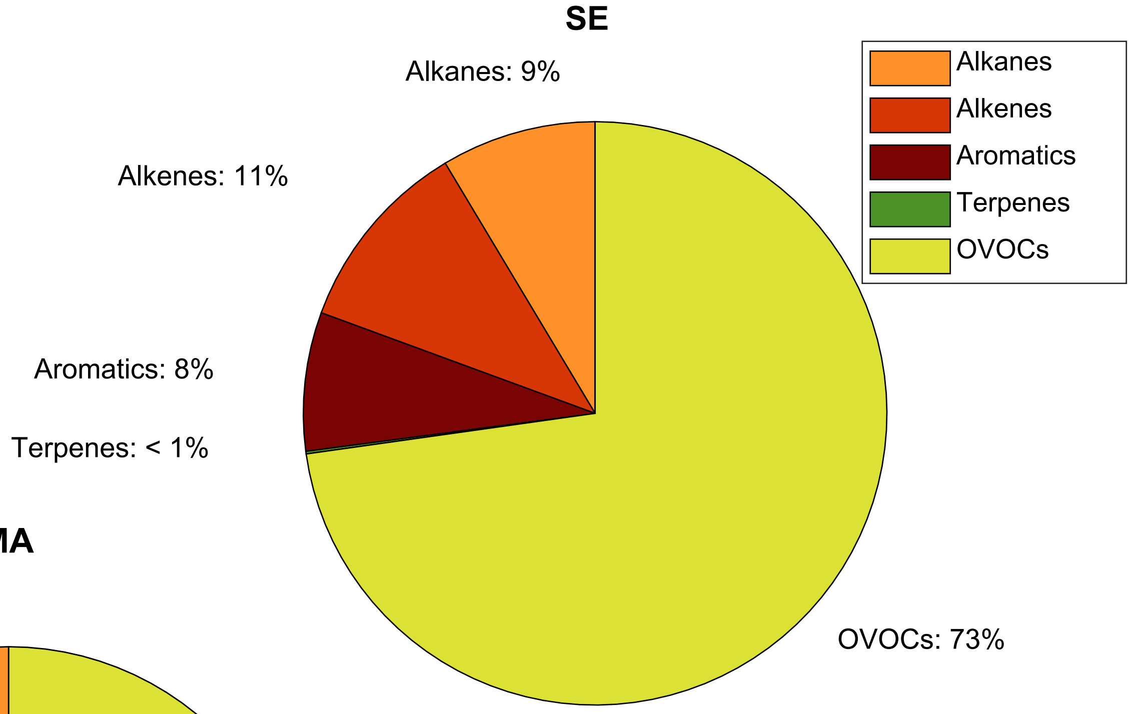
$$\mathbf{VOC\ reactivity} = \Sigma \mathbf{k_{OH+VOC}[OH][VOC]}$$



MM: mean VOCR = 3/s

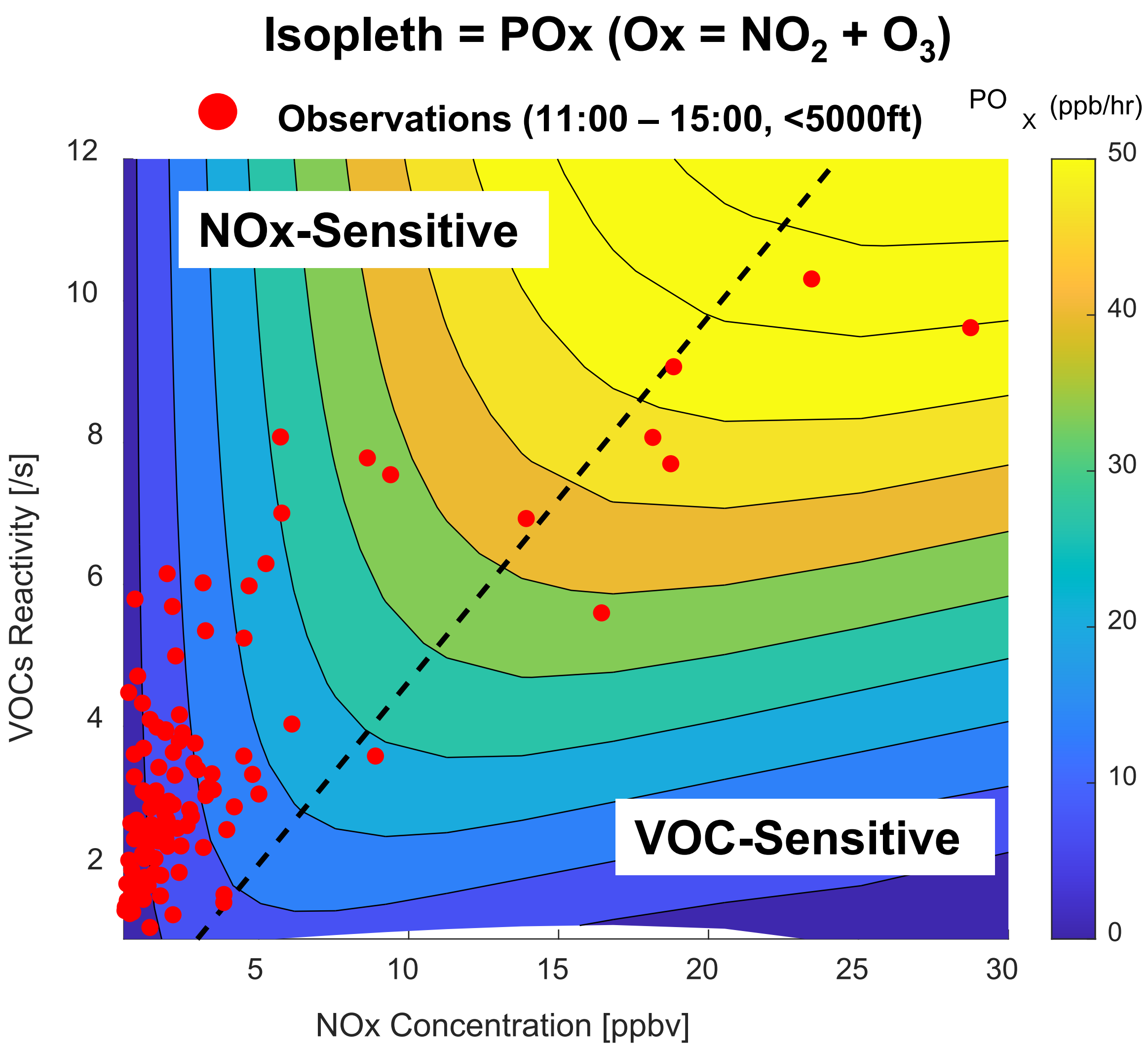


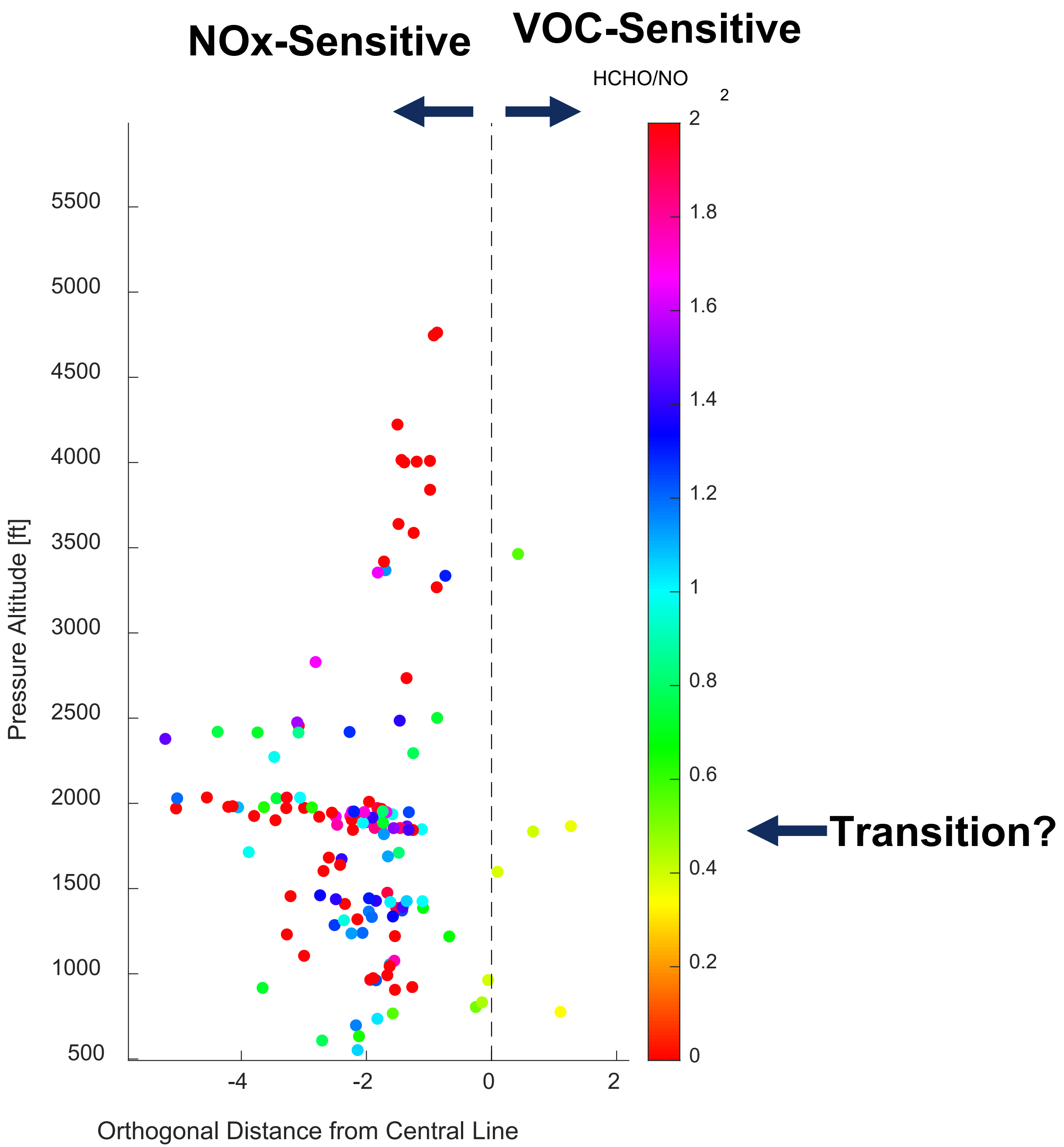
SMA: mean VOCR = 1.6/s



SE: mean VOCR = 1.2/s

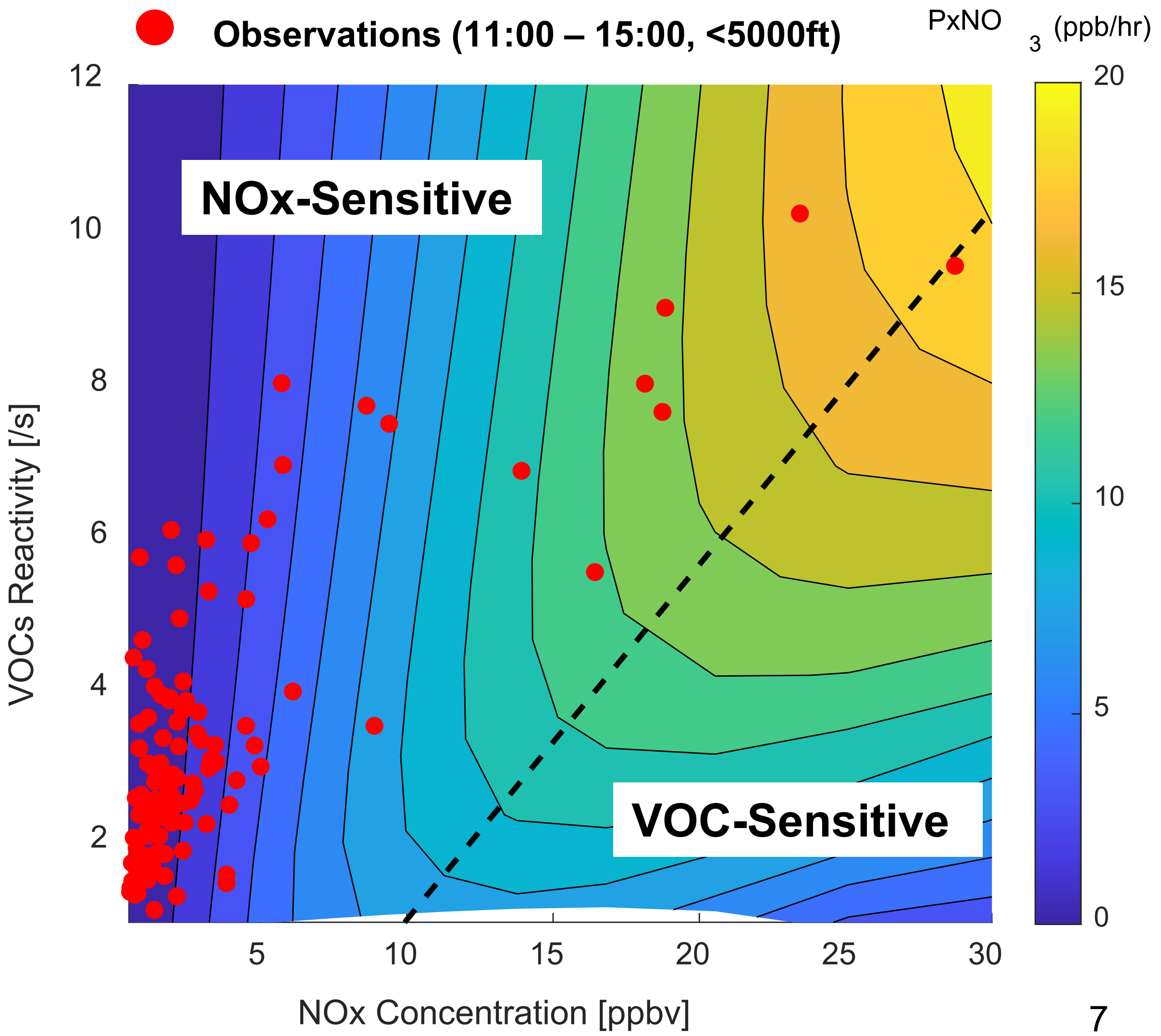
Box model results – MM (PHL)

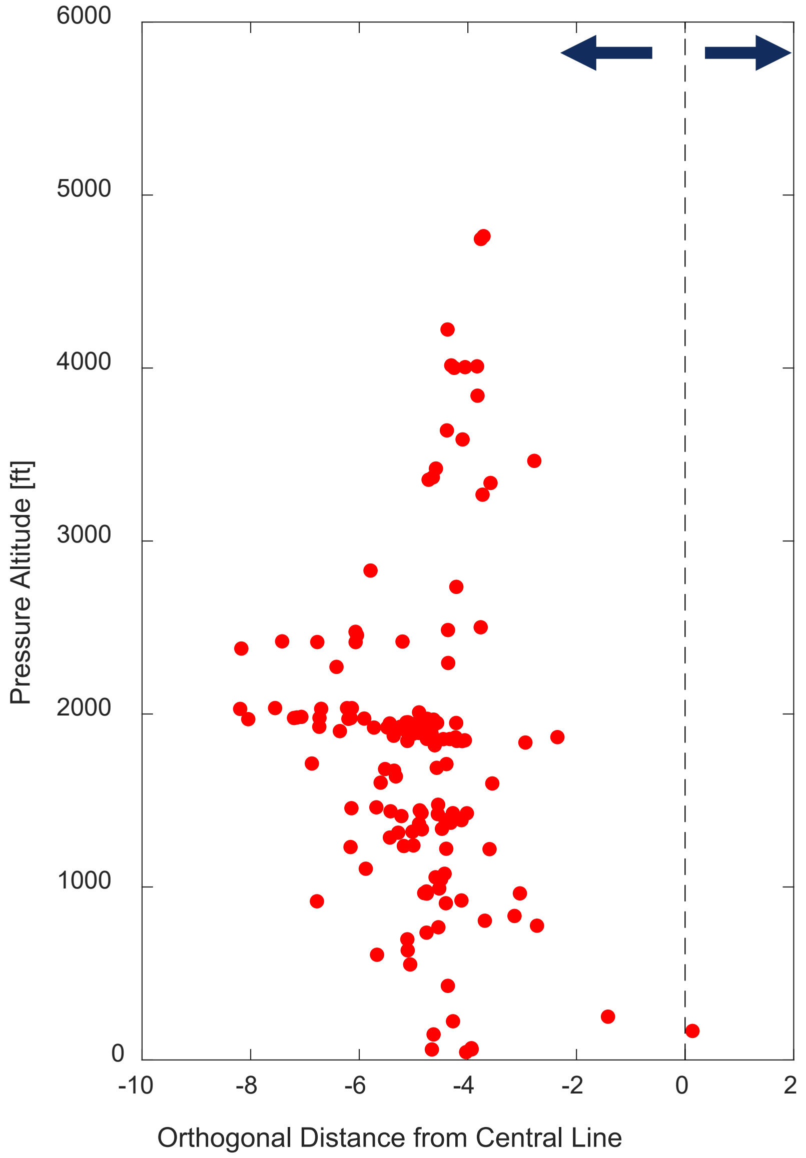




Box model results – MM (PHL)

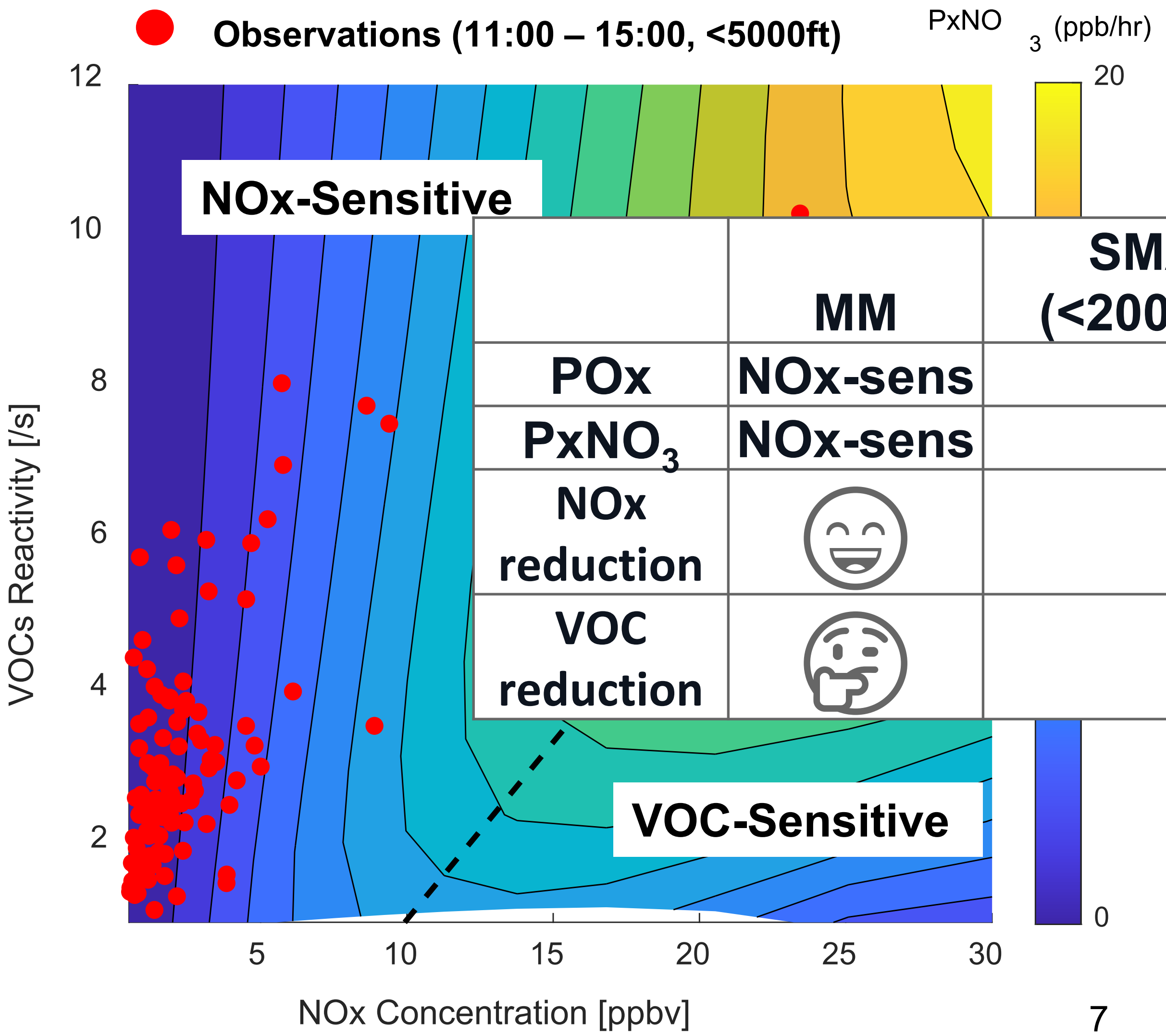
Isopleth = $PxNO_3$ ($xNO_3 = RONO_2(g)+HNO_3(g)+NO_3^-(aq)$)



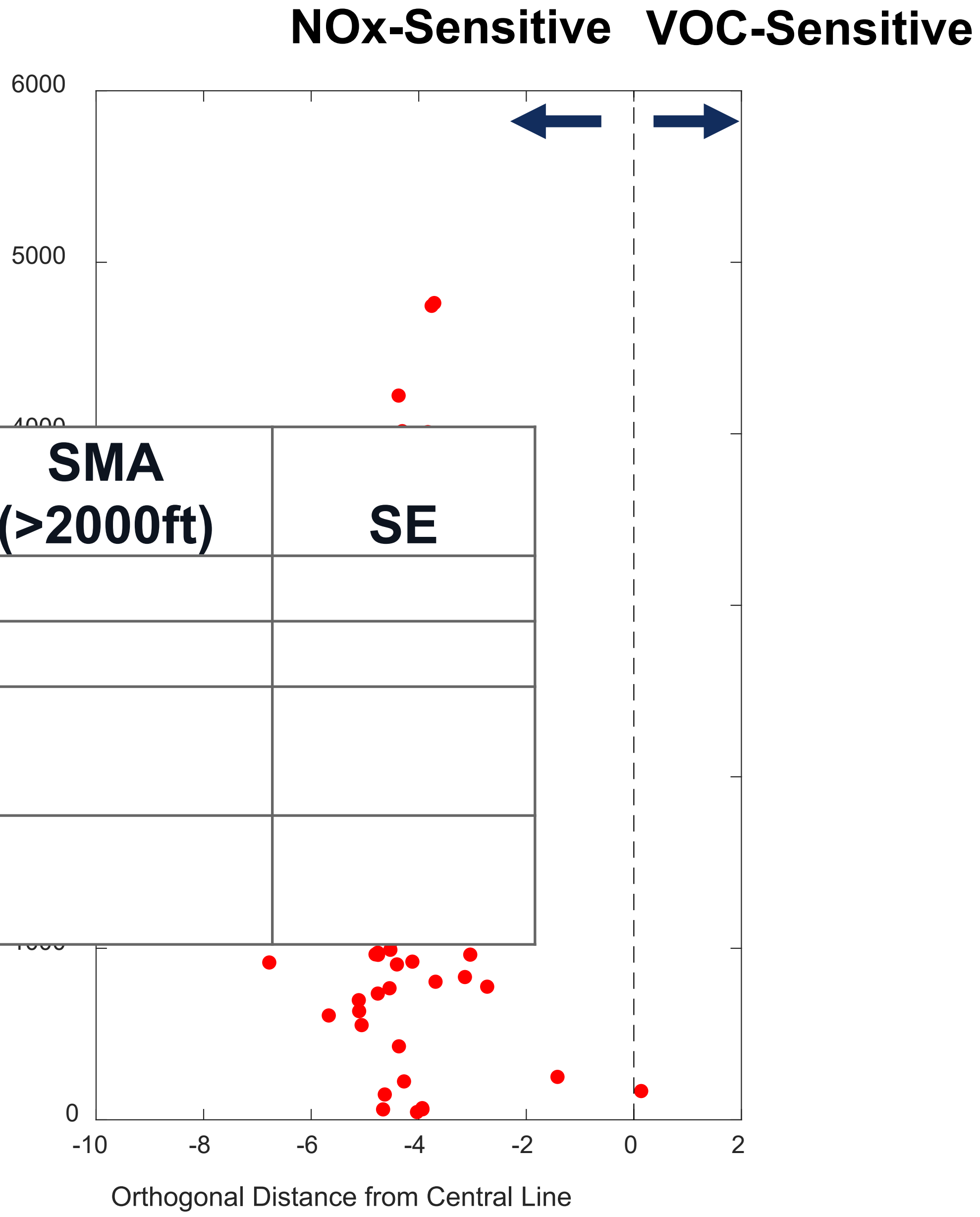


Box model results – MM (PHL)

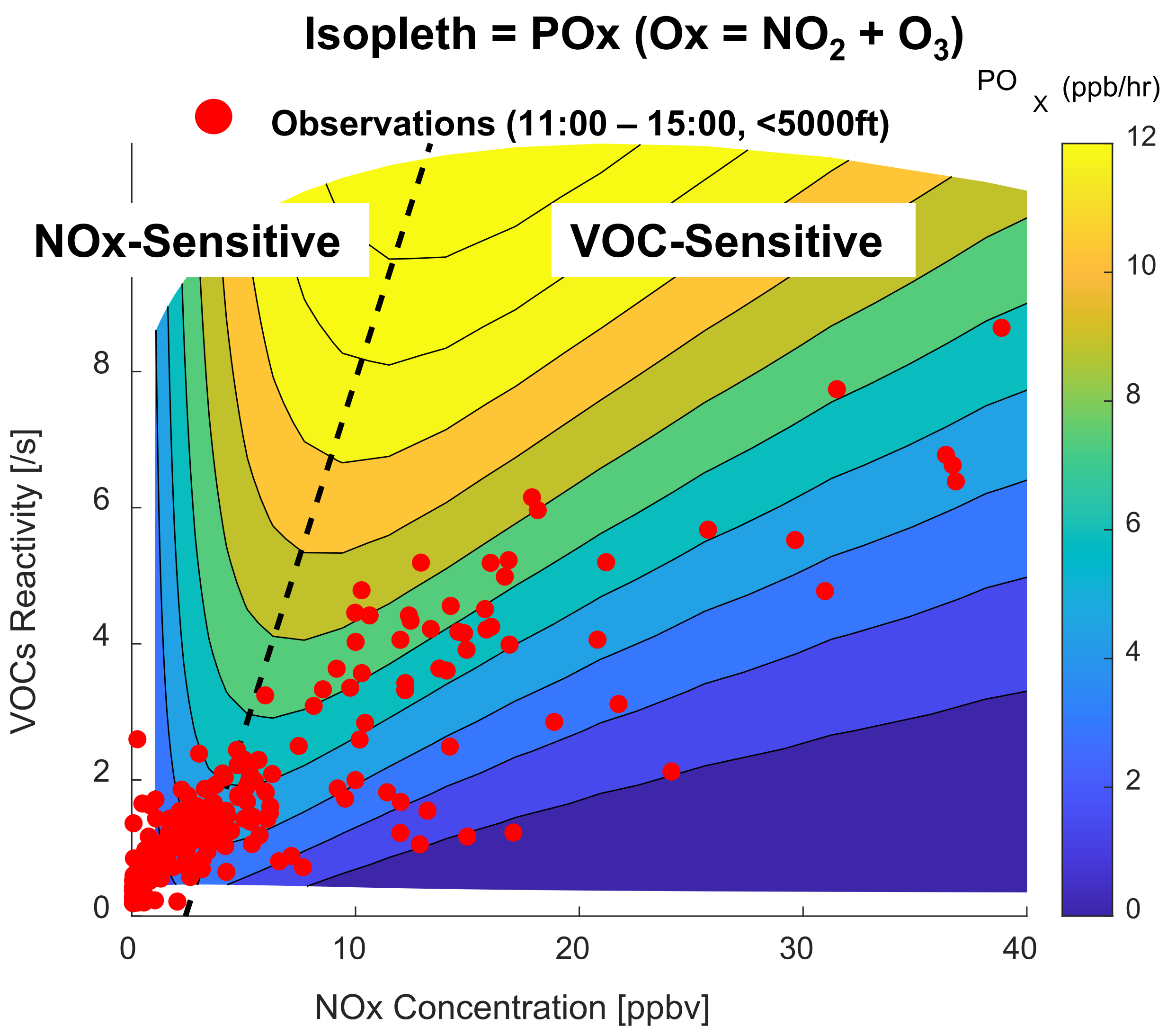
Isopleth = $PxNO_3$ ($xNO_3 = RONO_2(g)+HNO_3(g)+NO_3^-(aq)$)

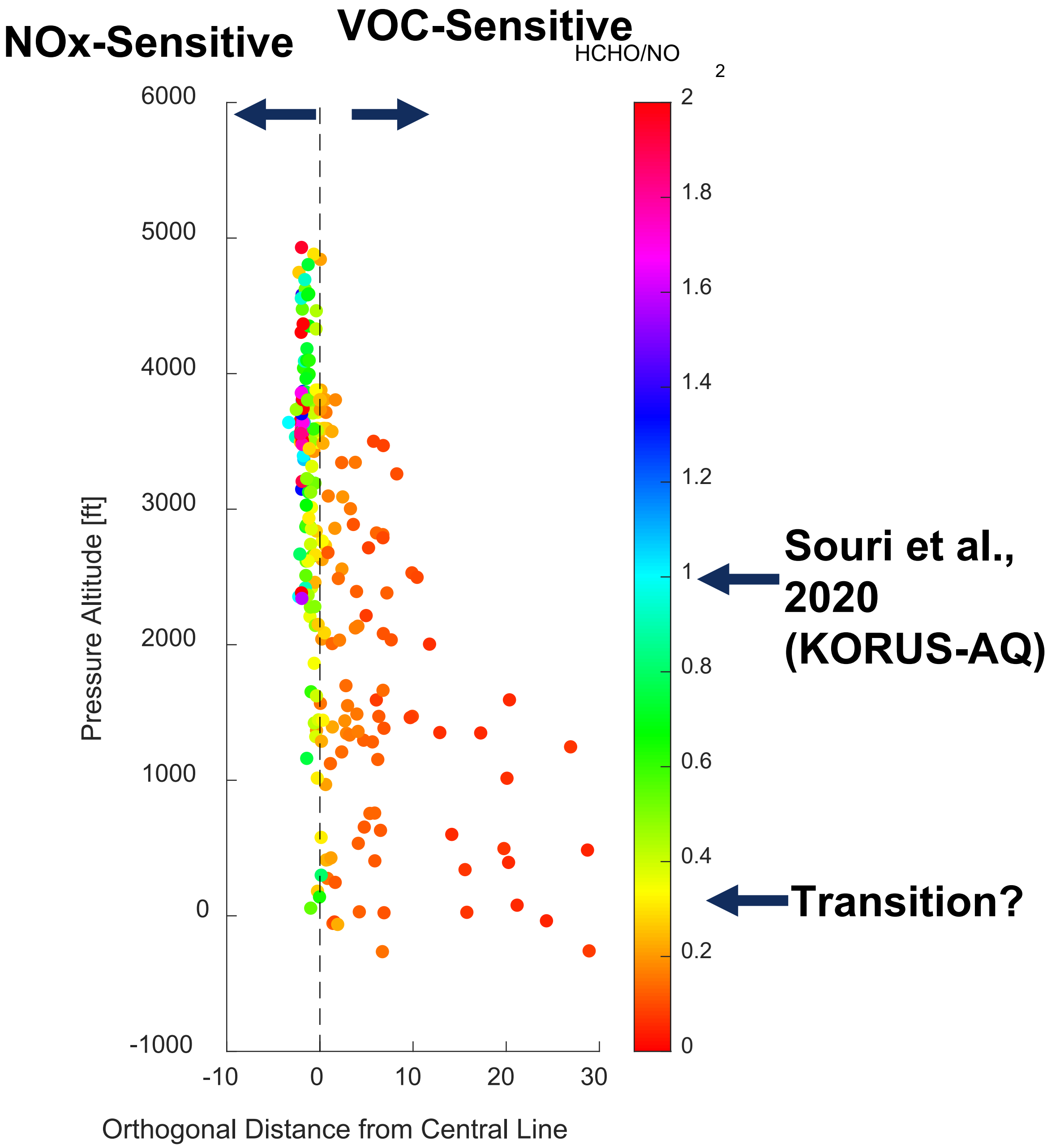


	MM	SMA (<2000ft)	SMA (>2000ft)	SE
POx	NOx-sens			
$PxNO_3$	NOx-sens			
NOx reduction	😄			
VOC reduction	🤔			



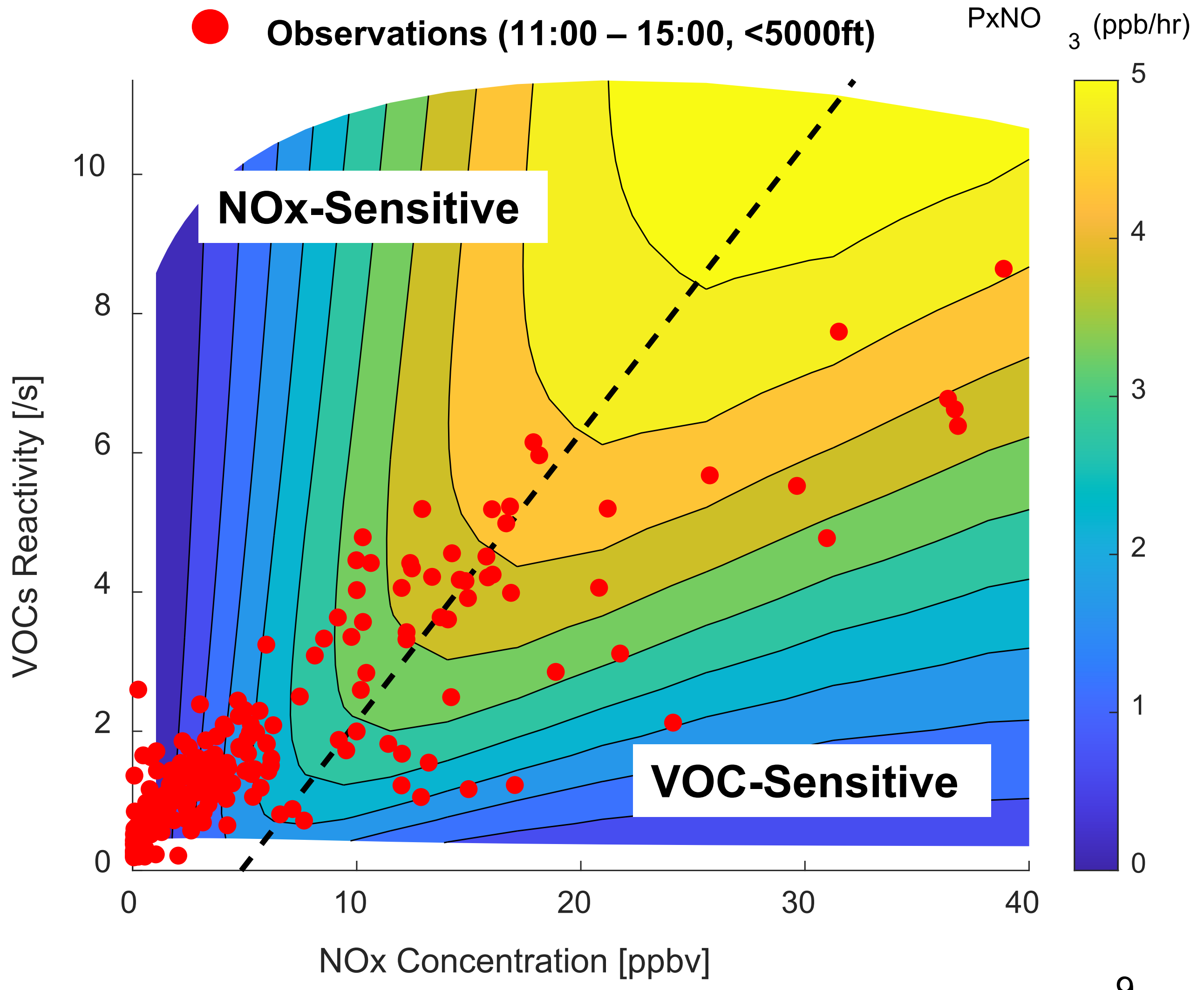
Box model results – SMA (KOR)

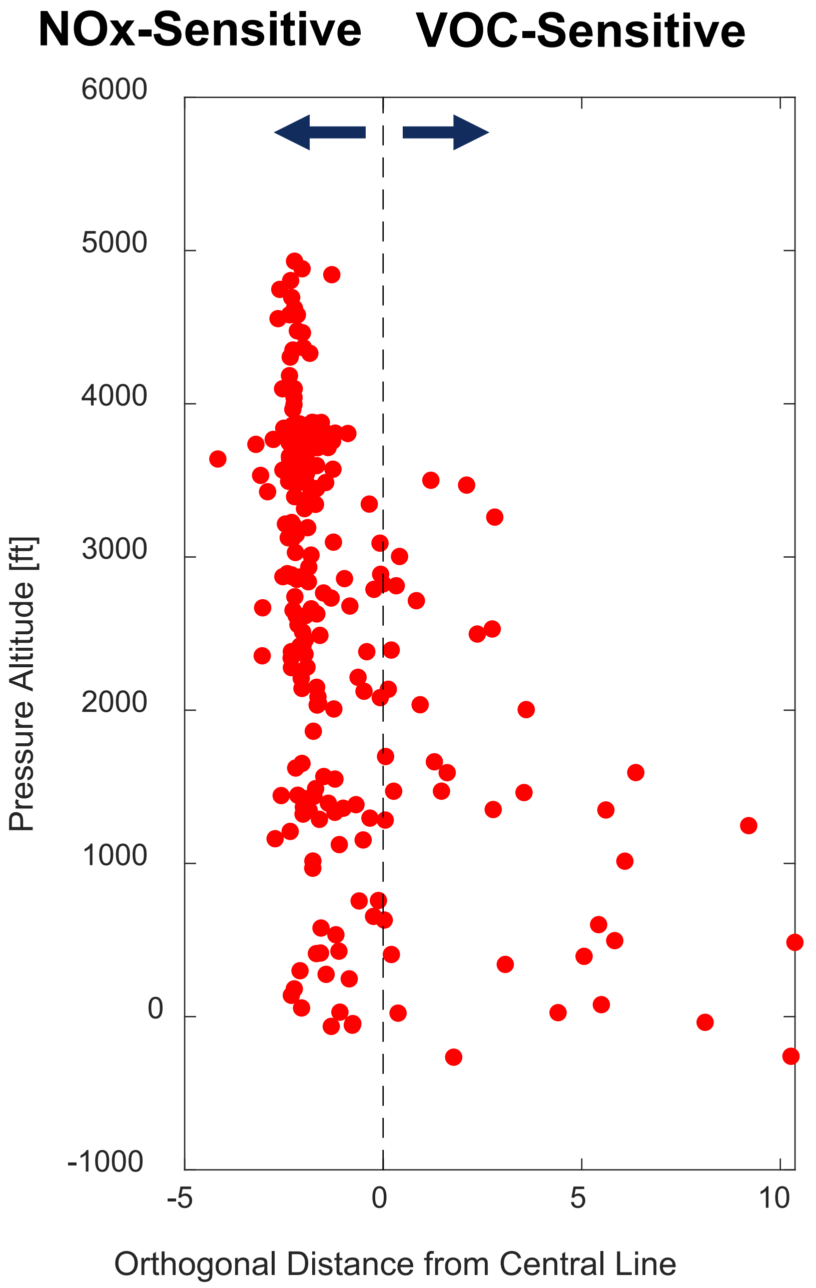




Box model results - SMA (KOR)

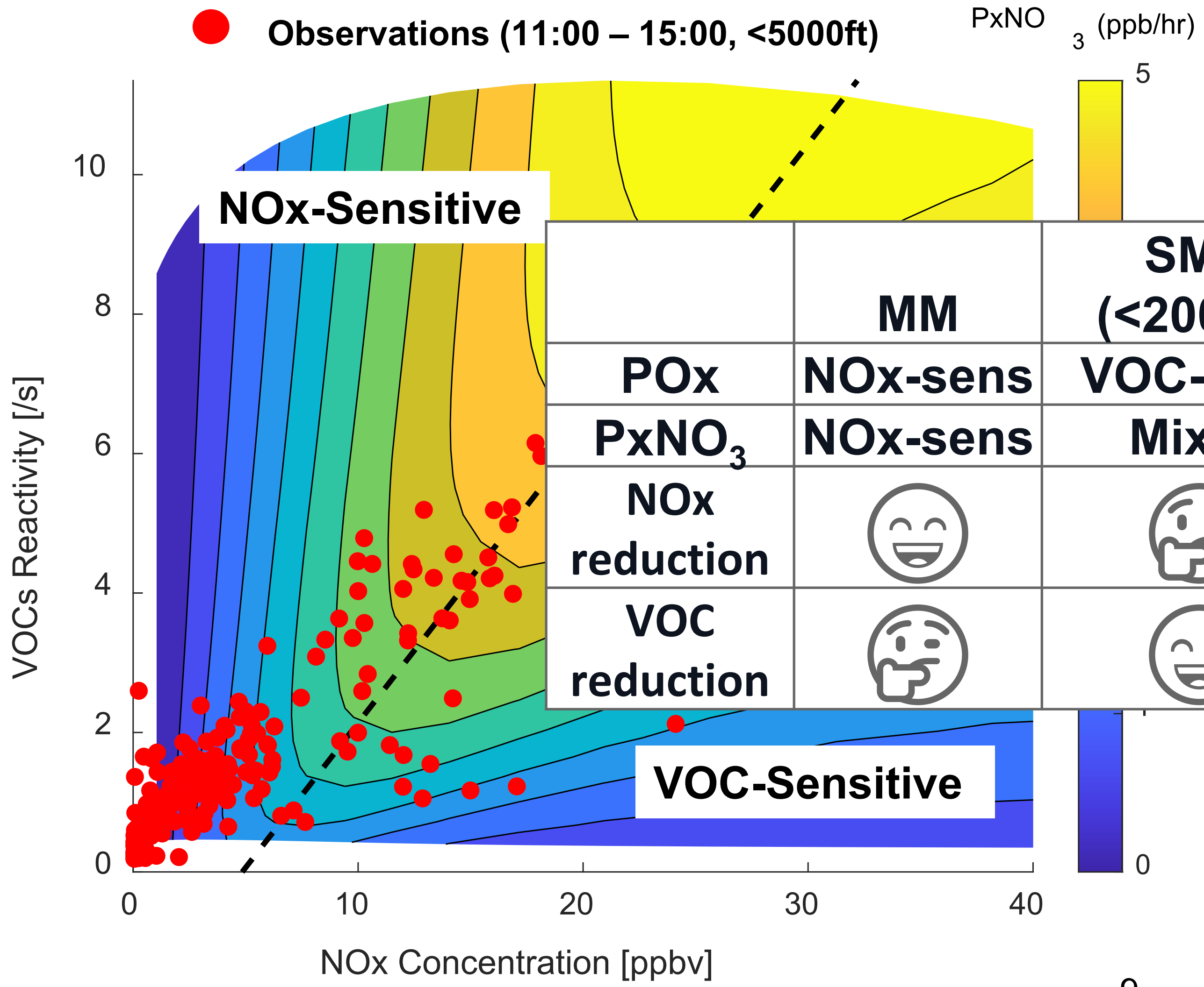
Isopleth = $PxNO_3$ ($xNO_3 = RONO_2(g)+HNO_3(g)+NO_3^-(aq)$)

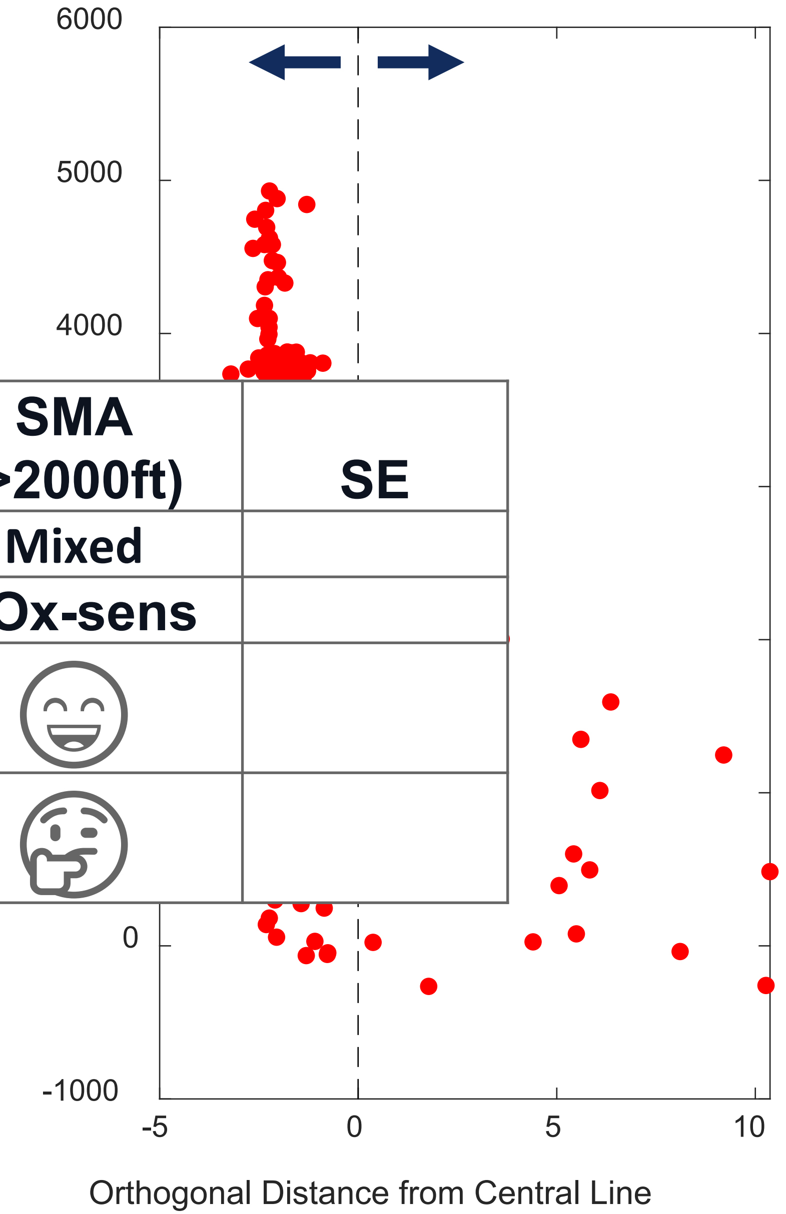




Box model results - SMA (KOR)

Isopleth = $PxNO_3$ ($xNO_3 = RONO_2(g) + HNO_3(g) + NO_3^-(aq)$)

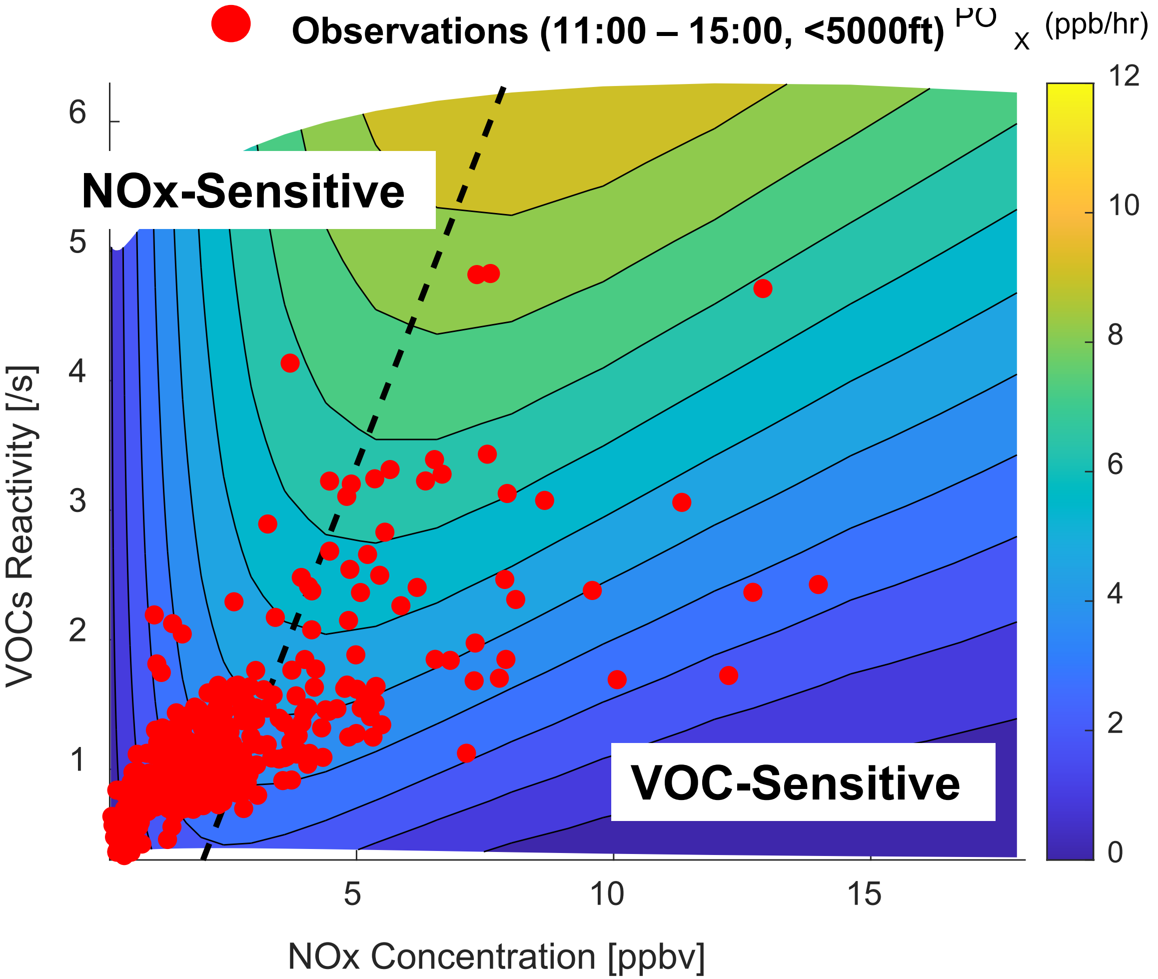


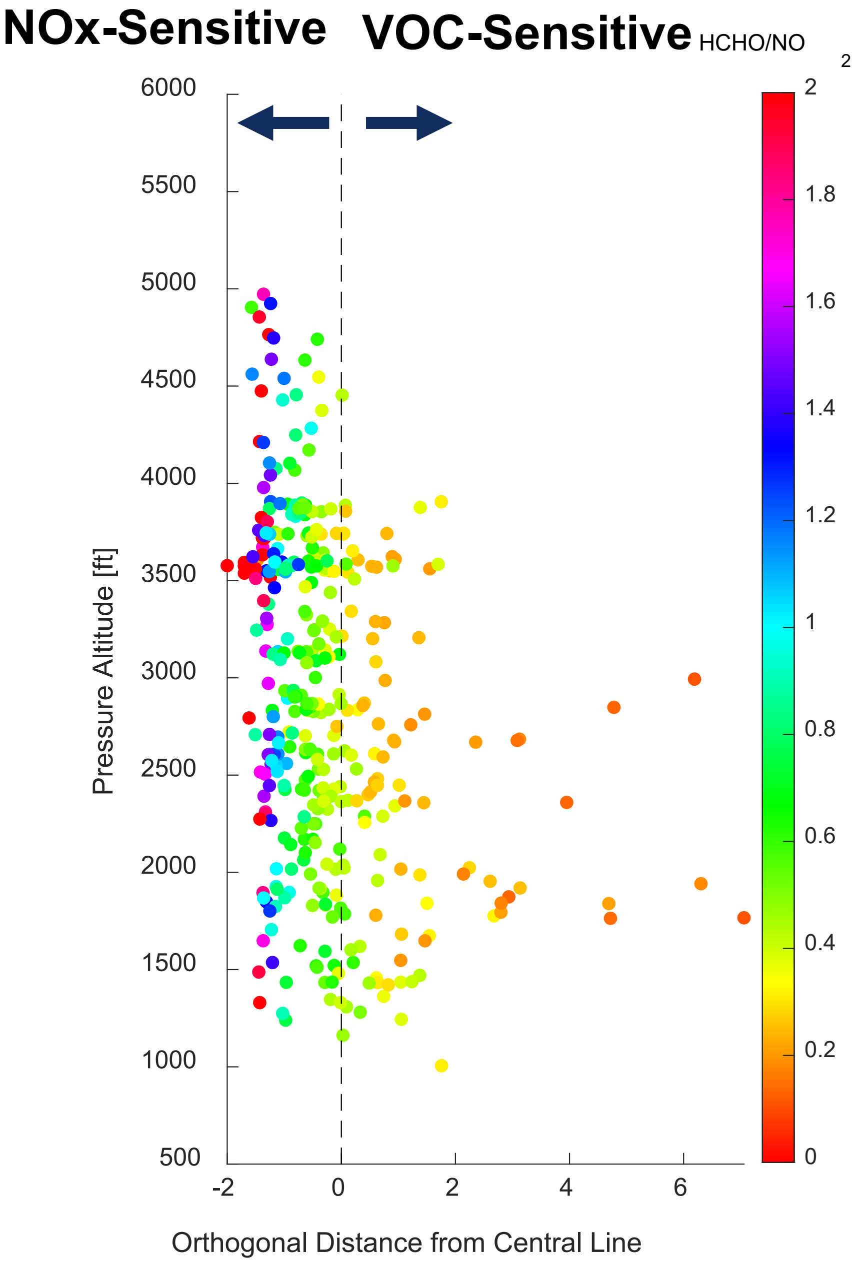


	MM	SMA (<2000ft)	SMA (>2000ft)	SE
POx	NOx-sens	VOC-sens	Mixed	
$PxNO_3$	NOx-sens	Mixed	NOx-sens	
NOx reduction	😄	🤔	😄	
VOC reduction	🤔	😄	🤔	

Box model results - SE (KOR)

Isopleth = POx (Ox = NO_2 + O_3)

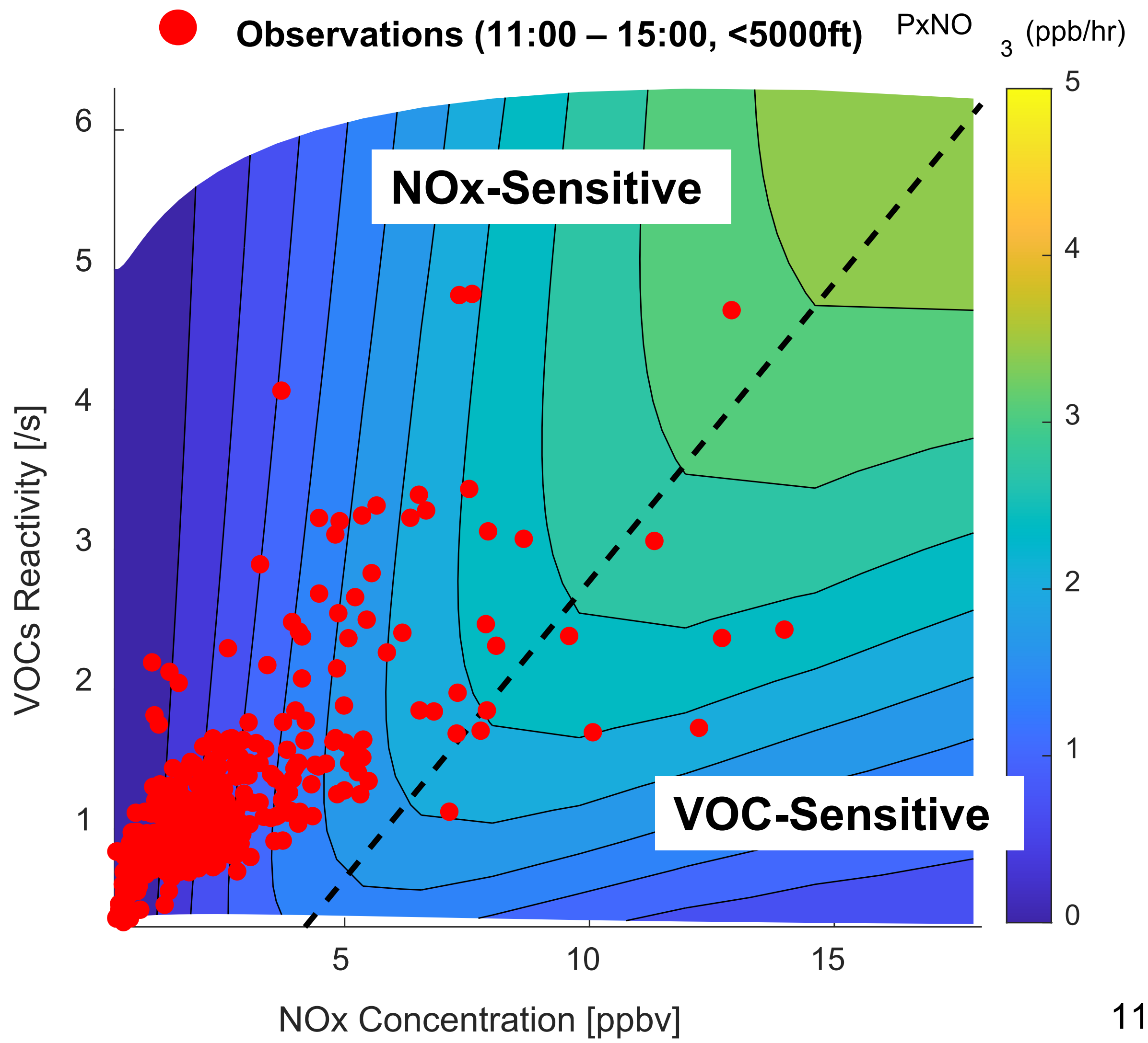


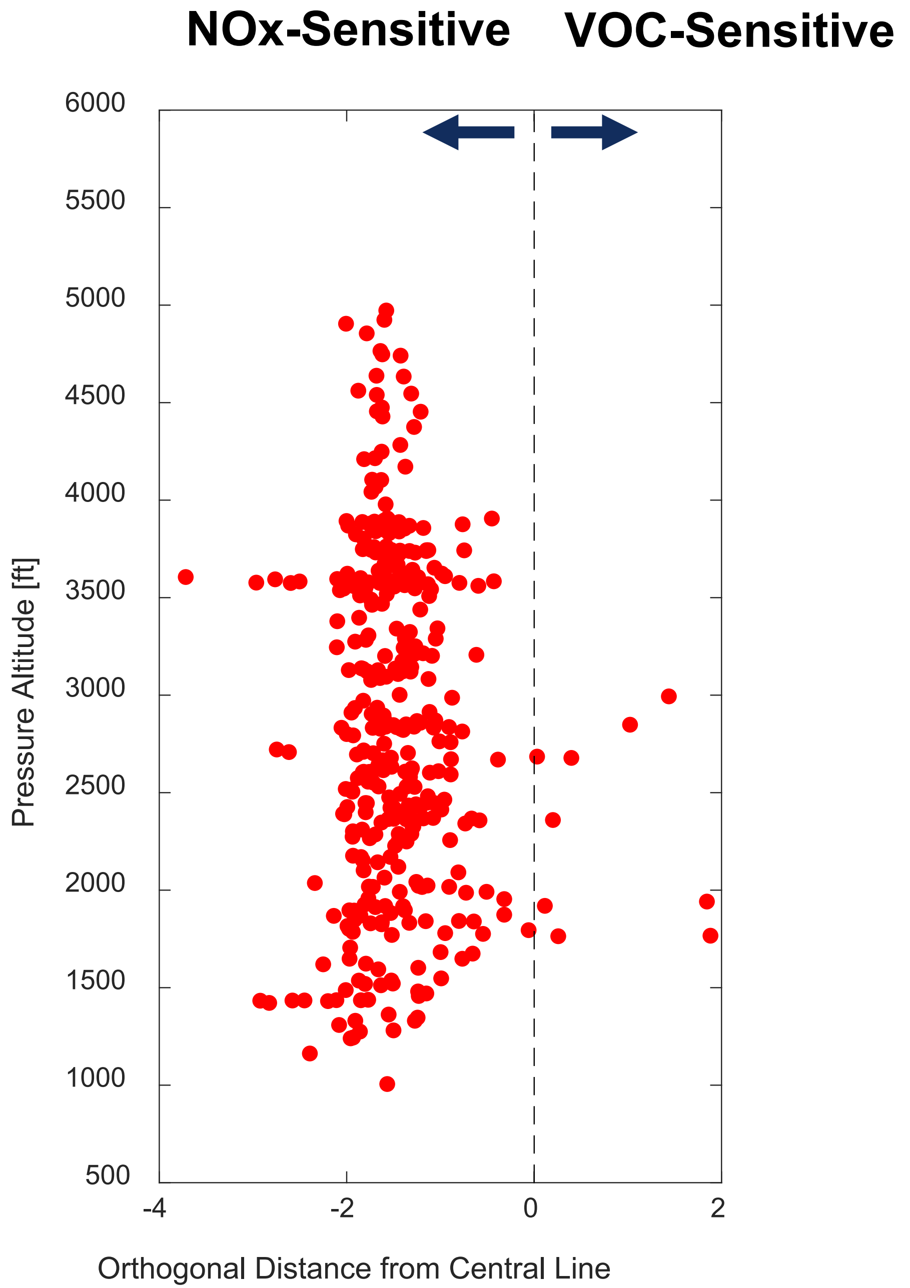


Transition?

Box model results - SE (KOR)

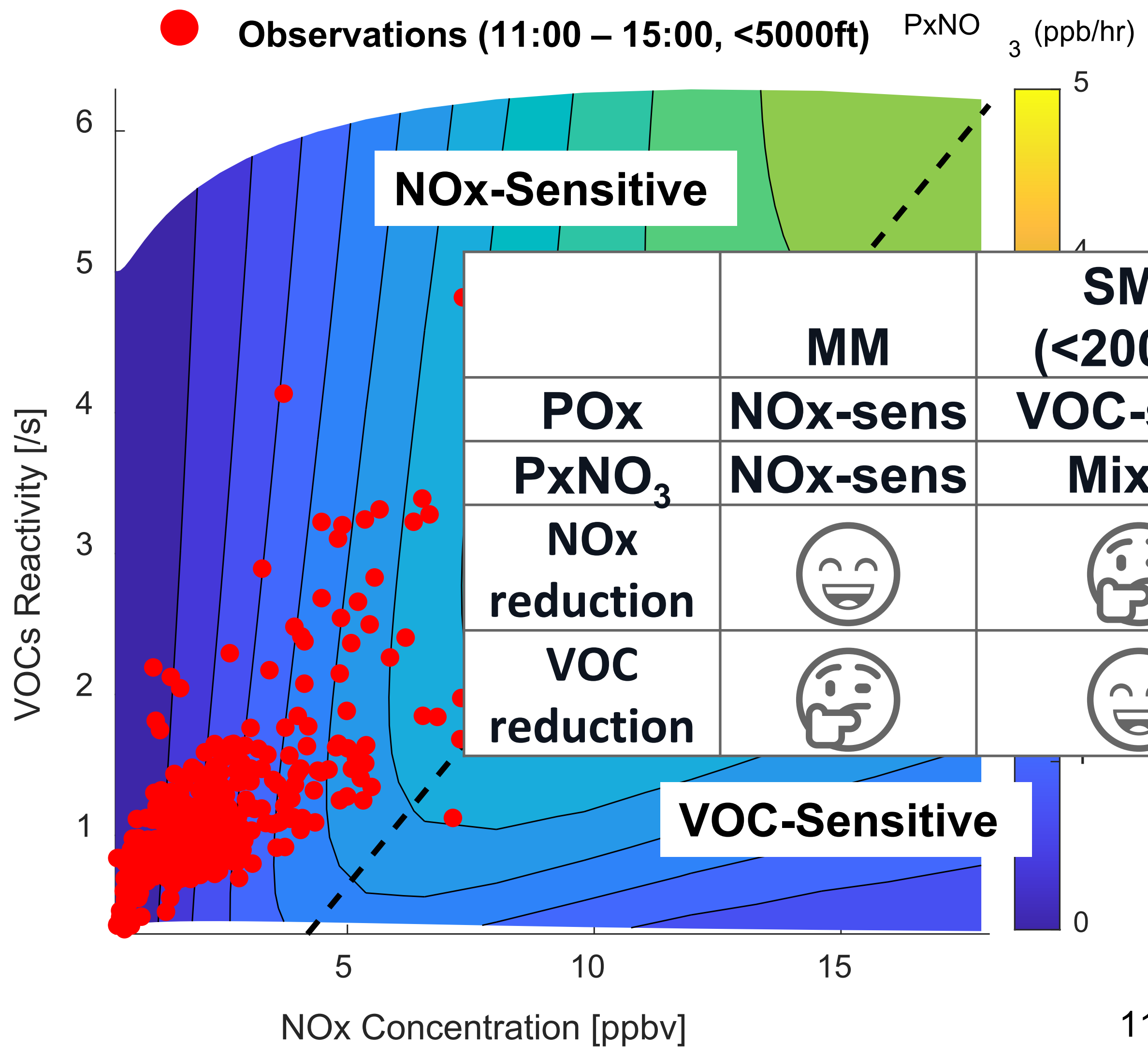
Isopleth = $PxNO_3$ ($xNO_3 = RONO_2(g)+HNO_3(g)+NO_3^-(aq)$)

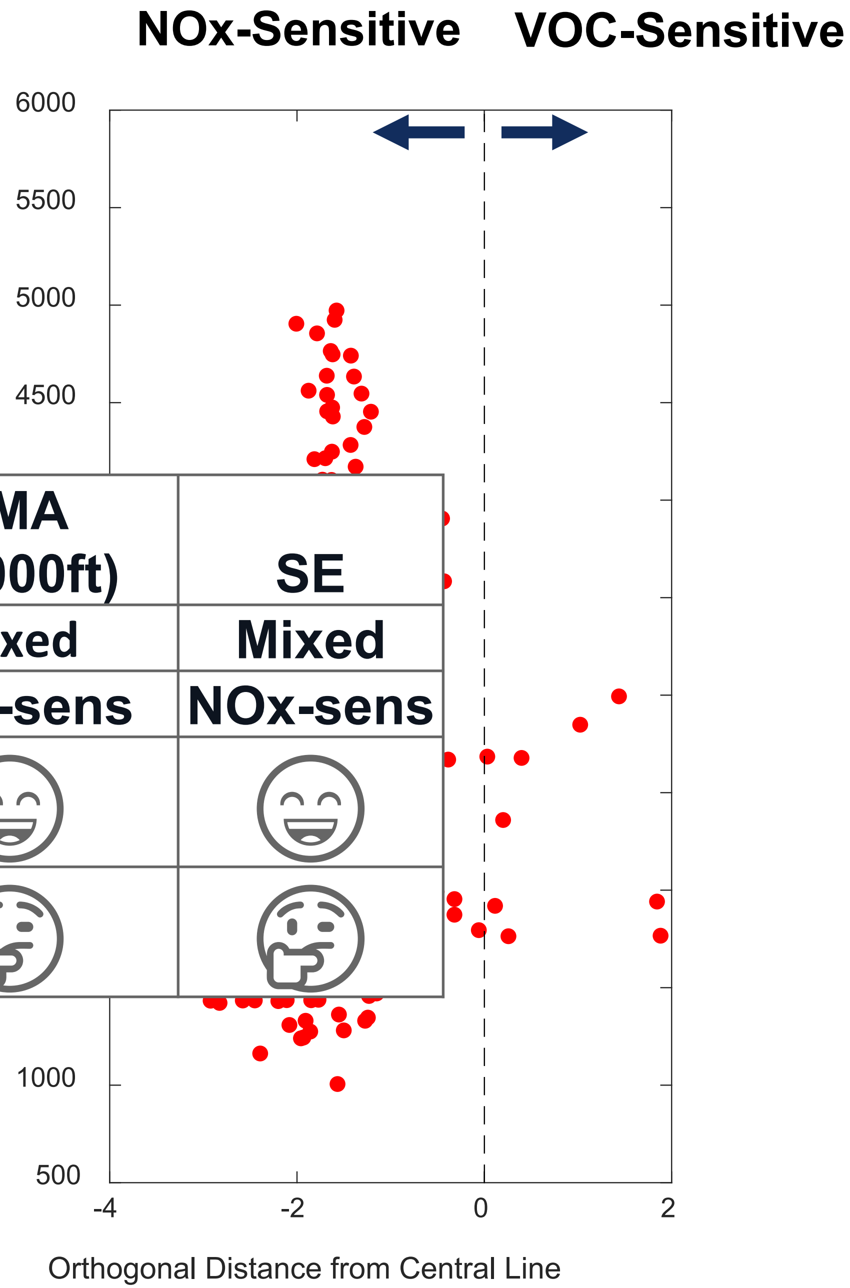




Box model results - SE (KOR)

Isopleth = $PxNO_3$ ($xNO_3 = RONO_2(g)+HNO_3(g)+NO_3^-(aq)$)





	MM	SMA (<2000ft)	SMA (>2000ft)	SE
POx	NOx-sens	VOC-sens	Mixed	Mixed
$PxNO_3$	NOx-sens	Mixed	NOx-sens	NOx-sens
NOx reduction	😄	🤔	😄	😄
VOC reduction	🤔	😄	🤔	🤔

Summary & Outlooks

- **Preliminary analysis on Ozone and Nitrate production sensitivities were performed**

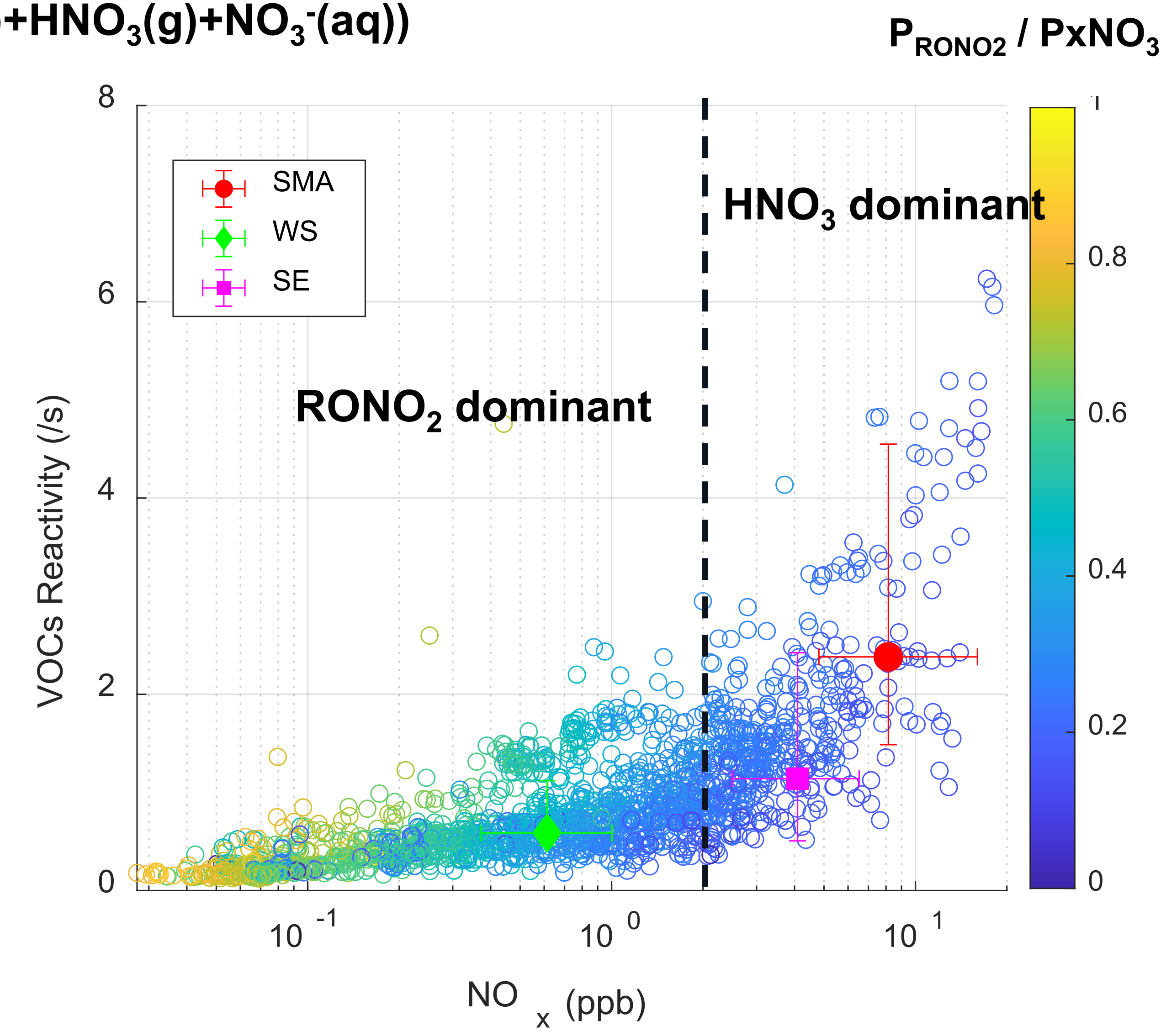
	MM	SMA (<2000ft)	SMA (>2000ft)	SE
POx	NOx-sens	VOC-sens	Mixed	Mixed
$PxNO_3$	NOx-sens	Mixed	NOx-sens	NOx-sens
NOx reduction	😄	🤔	😄	😄
VOC reduction	🤔	😄	🤔	🤔

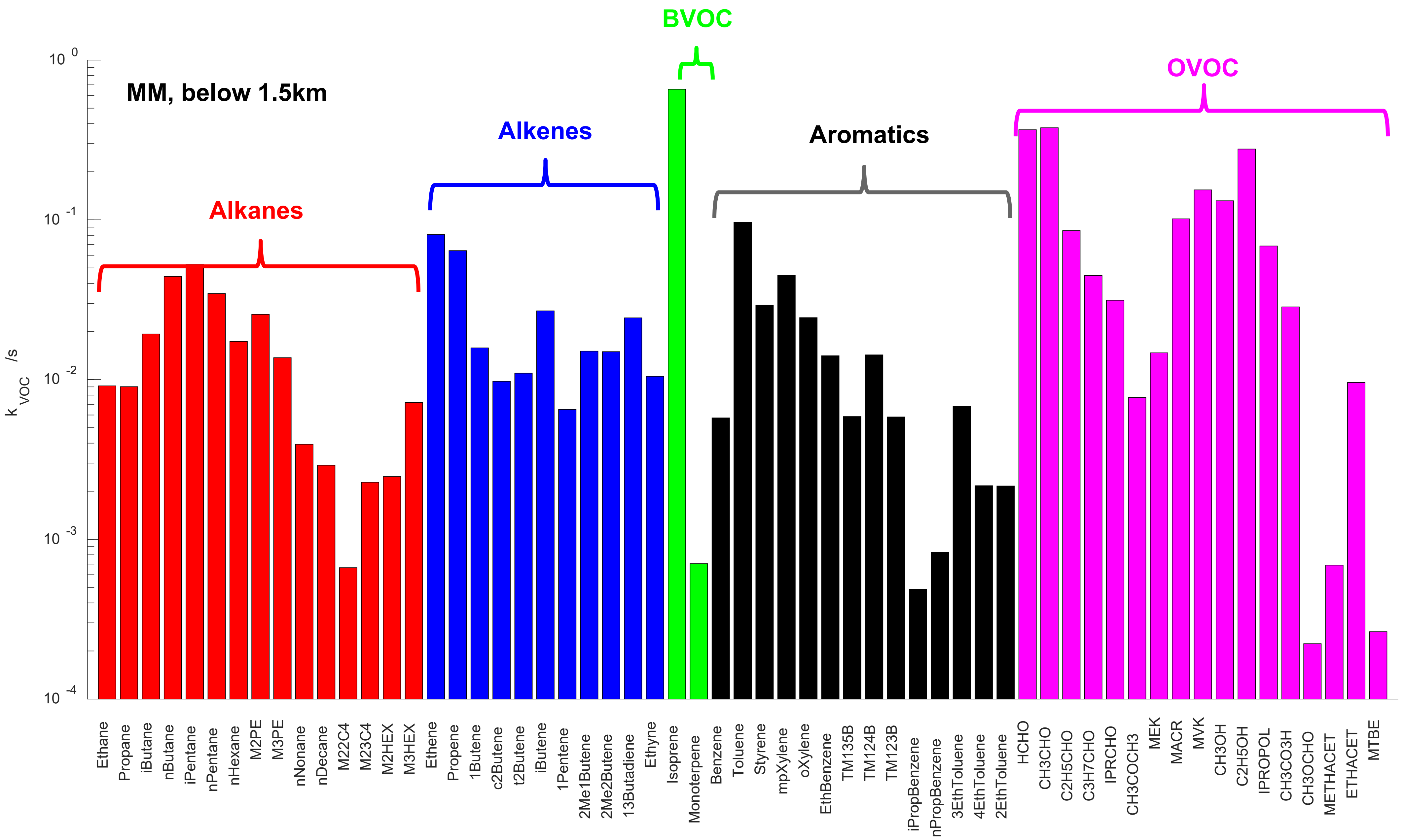
- **Transitions occurs in 0.3~0.5 $HCHO/NO_2$ (L_N/Q?)**
- **Ozone and Nitrate analysis in Taiwan and Thailand are in progress**
- **Sensitivity tests with different scenarios (e.g., VCP reduction)**
- **Comparison with KORUS-AQ (May to June, 2016)**
- **Look into $HNO_3 + NH_3 \leftrightarrow NH_4NO_3$ to differentiate gaseous and particulate nitrate production rates**

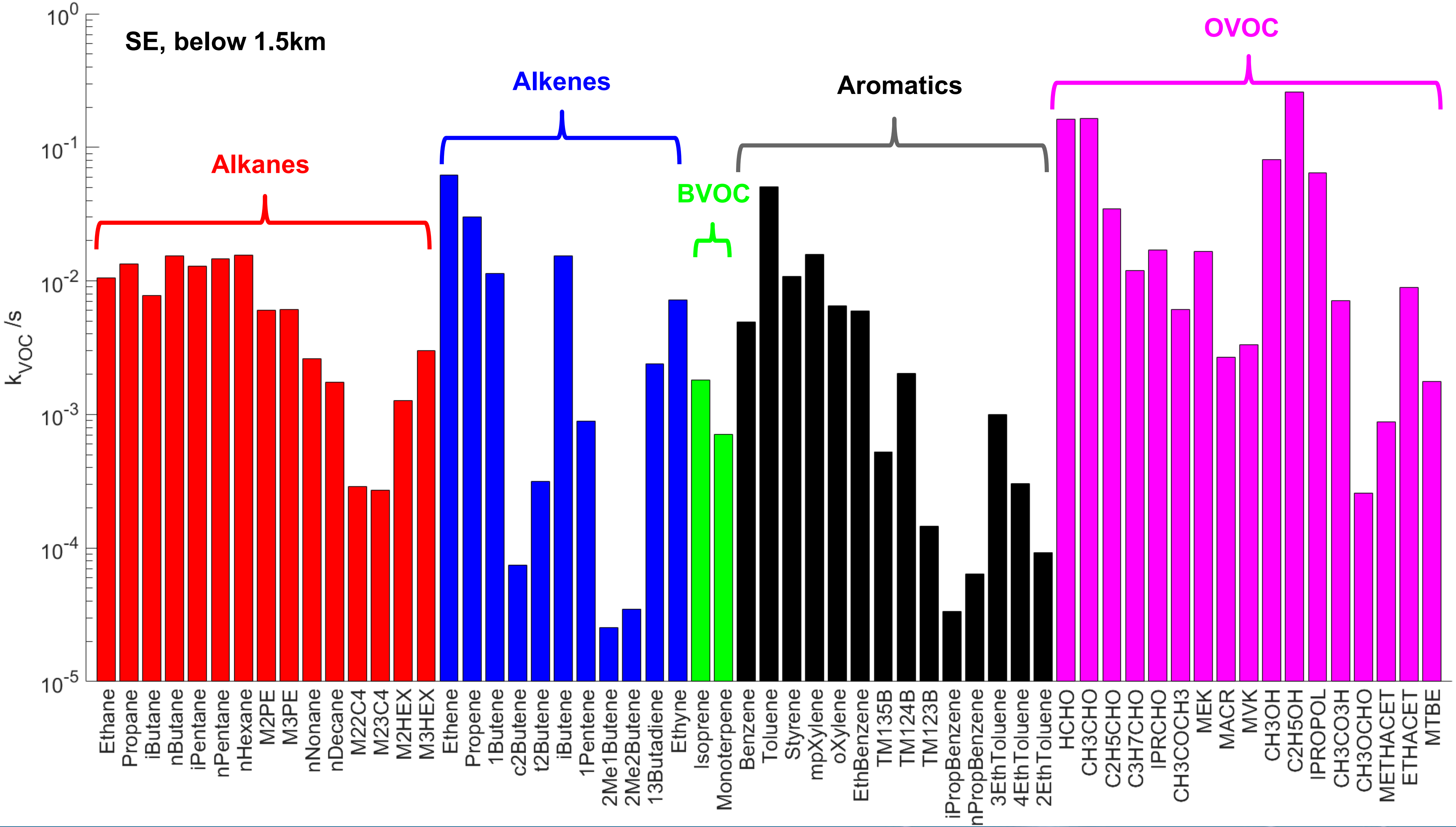
Thank you!

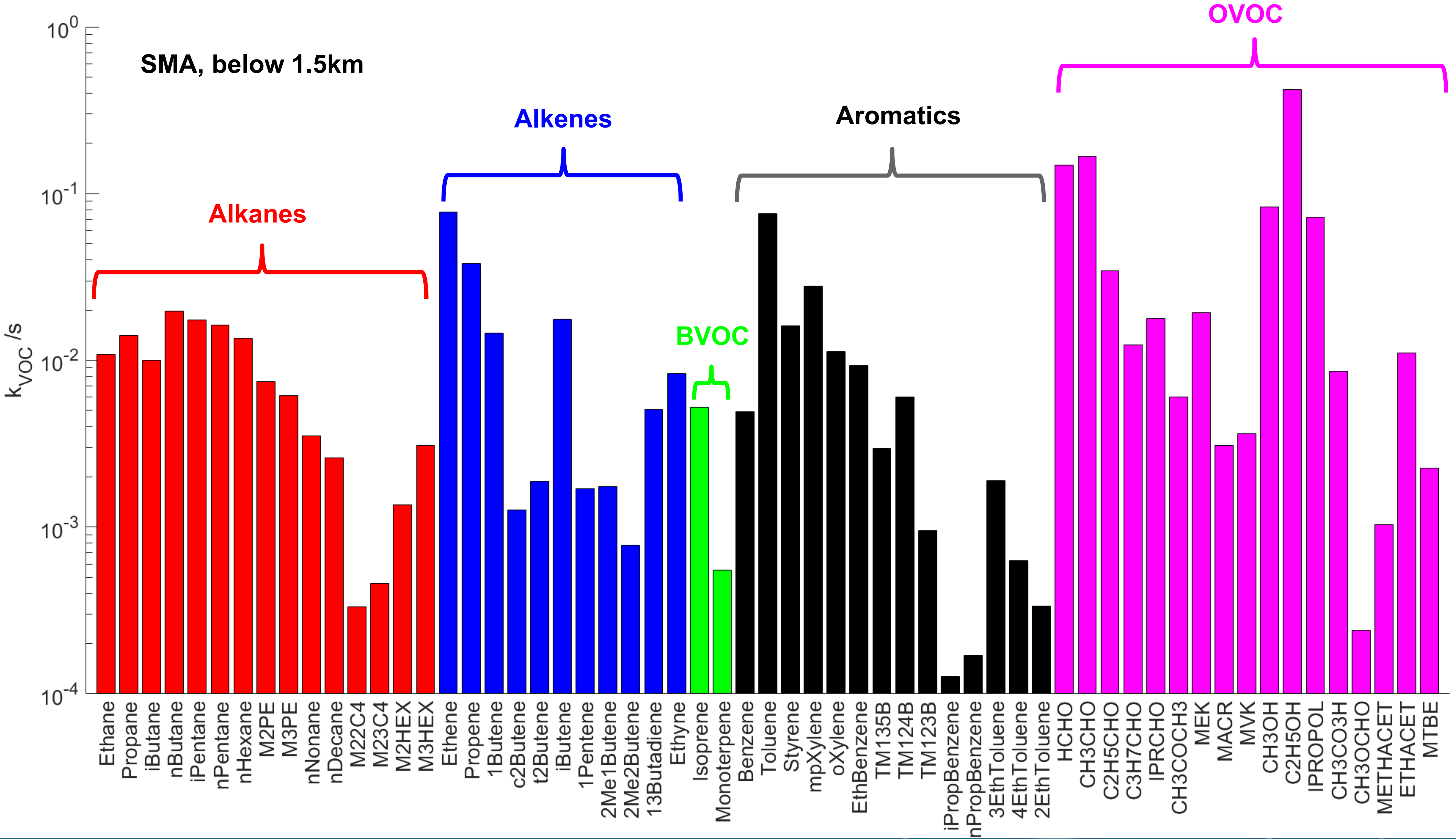
Box model results - KOR

$PxNO_3$ ($xNO_3 = RONO_2(g)+HNO_3(g)+NO_3^-(aq)$)

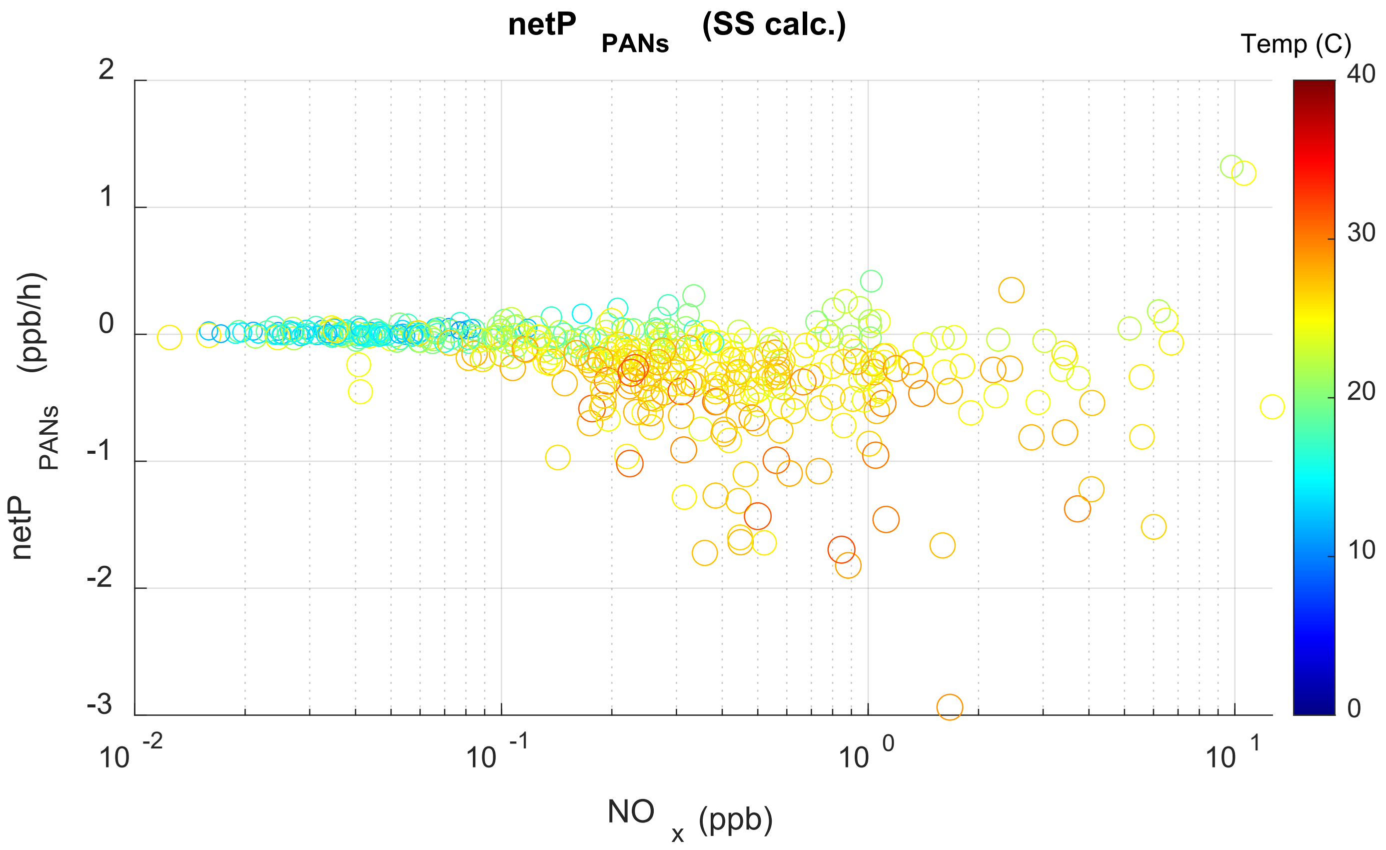



MM, below 1.5km
Alkanes
Alkenes
BVOC
Aromatics
OVOC
k VOC /s
10 0
10 -1
10 -2
10 -3
10 -4
Ethane
Propane
iButane
nButane
iPentane
nPentane
nHexane
M2PE
M3PE
nNonane
nDecane
M22C4
M23C4
M2HEX
M3HEX
Ethene
Propene
1Butene
c2Butene
t2Butene
iButene
1Pentene
2Me1Butene
2Me2Butene
13Butadiene
Ethyne
Isoprene
Monoterpene
Benzene
Toluene
Styrene
mpXylene
oXylene
EthBenzene
TM135B
TM124B
TM123B
iPropBenzene
nPropBenzene
3EthToluene
4EthToluene
2EthToluene
HCHO
CH3CHO
C2H5CHO
C3H7CHO
IPRCHO
CH3COCH3
MEK
MACR
MVK
CH3OH
C2H5OH
IPROPOL
CH3CO3H
CH3OCHO
METHACET
ETHACET
MTBE

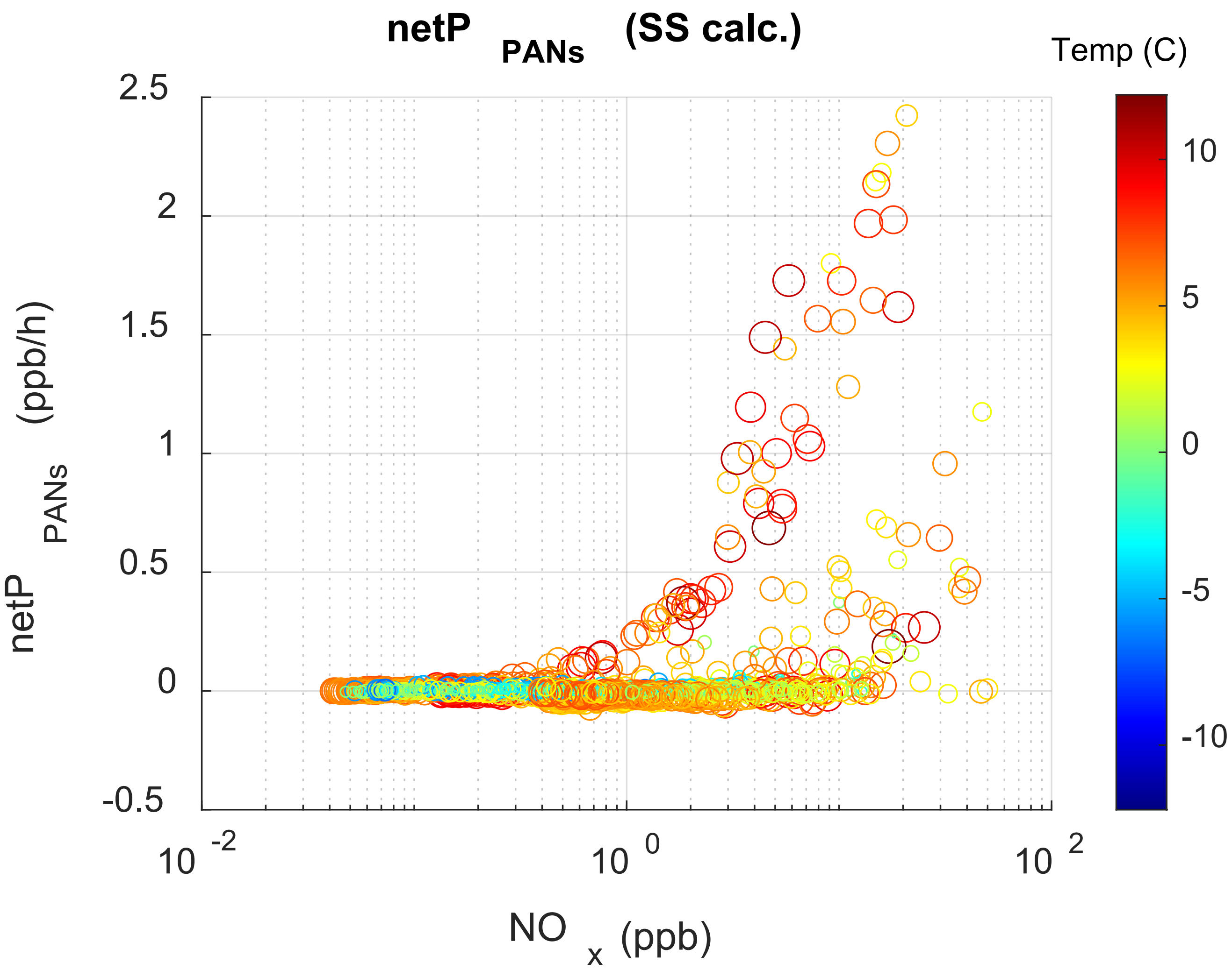

SE, below 1.5km
Alkanes
Alkenes
BVOC
Aromatics
OVOC
k_{VOC} /s
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
Ethane
Propane
iButane
nButane
iPentane
nPentane
nHexane
M2PE
M3PE
nNonane
nDecane
M22C4
M23C4
M2HEX
M3HEX
Ethene
Propene
1Butene
c2Butene
t2Butene
iButene
1Pentene
2Me1Butene
2Me2Butene
13Butadiene
Ethyne
Isoprene
Monoterpene
Benzene
Toluene
Styrene
mpXylene
oXylene
EthBenzene
TM135B
TM124B
TM123B
iPropBenzene
nPropBenzene
3EthToluene
4EthToluene
2EthToluene
HCHO
CH3CHO
C2H5CHO
C3H7CHO
IPRCHO
CH3COCH3
MEK
MACR
MVK
CH3OH
C2H5OH
IPROPOL
CH3CO3H
CH3OCHO
METHACET
ETHACET
MTBE


SMA, below 1.5km
Alkanes
Alkenes
BVOC
Aromatics
OVOC
k_{VOC} /s
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
Ethane
Propane
iButane
nButane
iPentane
nPentane
nHexane
M2PE
M3PE
nNonane
nDecane
M22C4
M23C4
M2HEX
M3HEX
Ethene
Propene
1Butene
c2Butene
t2Butene
iButene
1Pentene
2Me1Butene
2Me2Butene
13Butadiene
Ethyne
Isoprene
Monoterpene
Benzene
Toluene
Styrene
mpXylene
oXylene
EthBenzene
TM135B
TM124B
TM123B
iPropBenzene
nPropBenzene
3EthToluene
4EthToluene
2EthToluene
HCHO
CH3CHO
C2H5CHO
C3H7CHO
IPRCHO
CH3COCH3
MEK
MACR
MVK
CH3OH
C2H5OH
IPROPOL
CH3CO3H
CH3OCHO
METHACET
ETHACET
MTBE

Philippines



Korea


netP PANs (SS calc.)
Temp (C)
2.5
2
1.5
1
0.5
0
-0.5
netP PANs (ppb/h)
10 -2
10 0
10 2
NO x (ppb)
10
5
0
-5
-10

Ground Measurements of VOCs in Seoul during the ASIA-AQ Campaign

Joo-Ae Kim[a)],

Sohyeon Kang[a)], Meehye Lee[a)], Yuri Choi[b)], Romertta Kim[c)]

[a)]Department of Earth and Environmental Sciences, Korea University

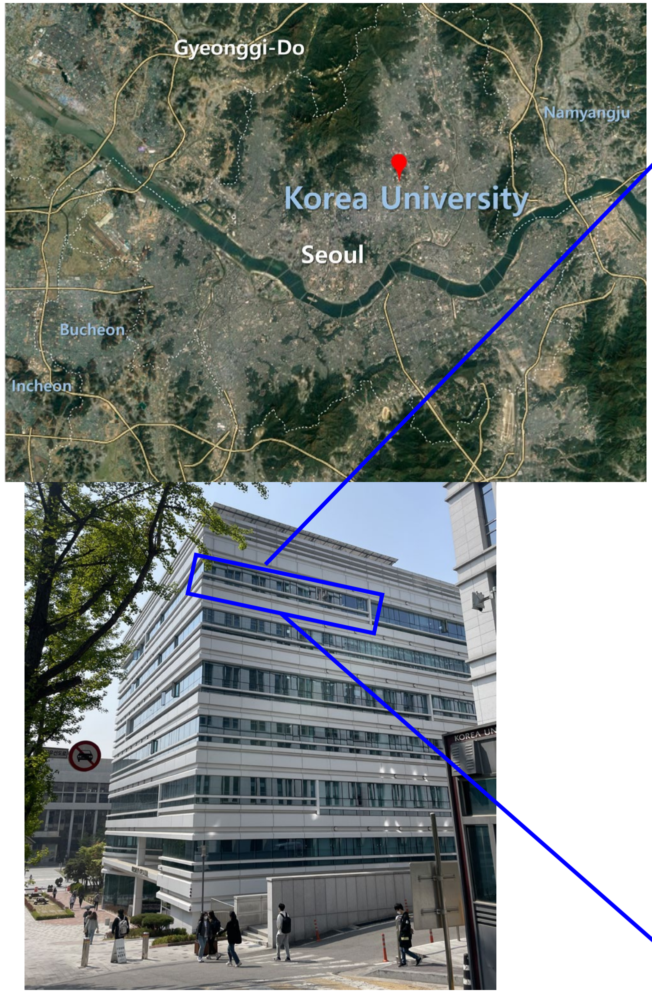
[b)]Seoul Government Research Institute of Health and Environment

[c)]Syft Technologies, Korea

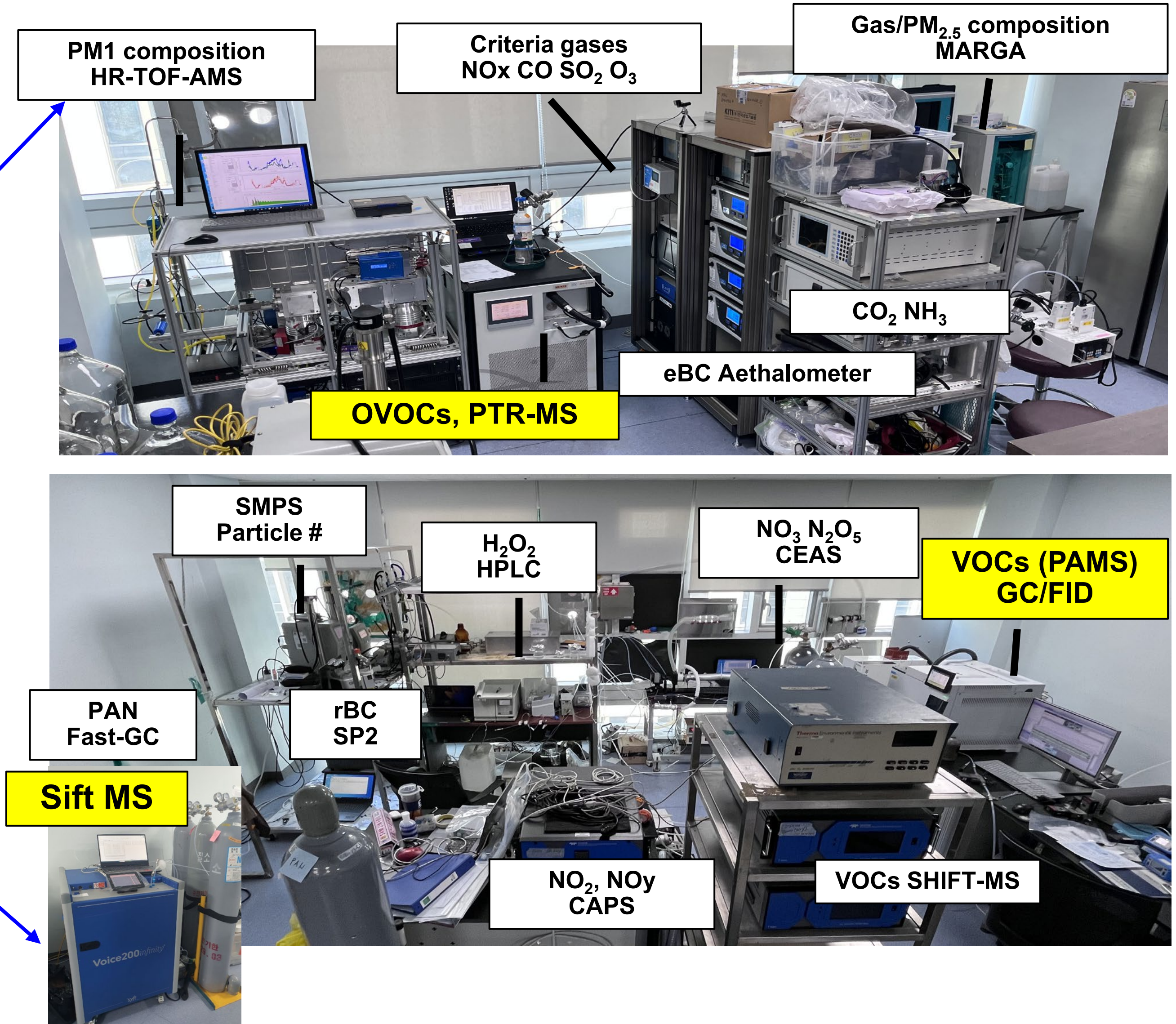
Ground Measurements

Site : Mediheal EES building, Korea University, Seoul (37.585ºN, 127.026ºE)

Period : 25th January ~ 27th March, 2024



Mediheal EES building in KU



VOCs Species

TD-GC-FID (PAMS)

compounds	type	compounds	type
ethane	alkane	23dimethylpentane	alkane
ethylene	alkene	3methylhexane	alkane
propane	alkane	224trimethylpentane	alkane
propylene	alkene	heptane	alkane
isobutane	alkane	methylcyclohexane	alkane
butane	alkane	234trimethylpentane	alkane
acetylene	alkyne	toluene	aromatic
trans2butene	alkene	2methylheptane	alkane
1butene	alkene	3methylheptane	alkane
cis2butene	alkene	octane	alkane
cyclopentane	alkane	ethylbenzene	aromatic
isopentane	alkane	mpxylene	aromatic
pentane	alkane	stylene	aromatic
trans2pentene	alkene	oxylene	aromatic
1pentene	alkene	nonane	alkane
cis2pentene	alkene	isopropylbenzene	aromatic
22dimethylbutane	alkane	propylbenzene	aromatic
23dimethylbutane	alkane	methyltoluene	aromatic
2methylpentane	alkane	pethyltoluene	aromatic
3methylpentane	alkane	135trimethylbenzene	aromatic
isoprene	alkene	oethyltoluene	aromatic
1hexene	alkene	124trimethylbenzene	aromatic
hexane	alkane	decane	alkane
methylcyclopentane	alkane	123trimethylbenzene	aromatic
24dimethylpentane	alkane	mdiethylbenzene	aromatic
benzene	aromatic	pdiethylbenzene	aromatic
cyclohexane	alkane	undecane	alkane
2methylhexane	alkane	dodecane	alkane

PTR-MS (OVOCs)

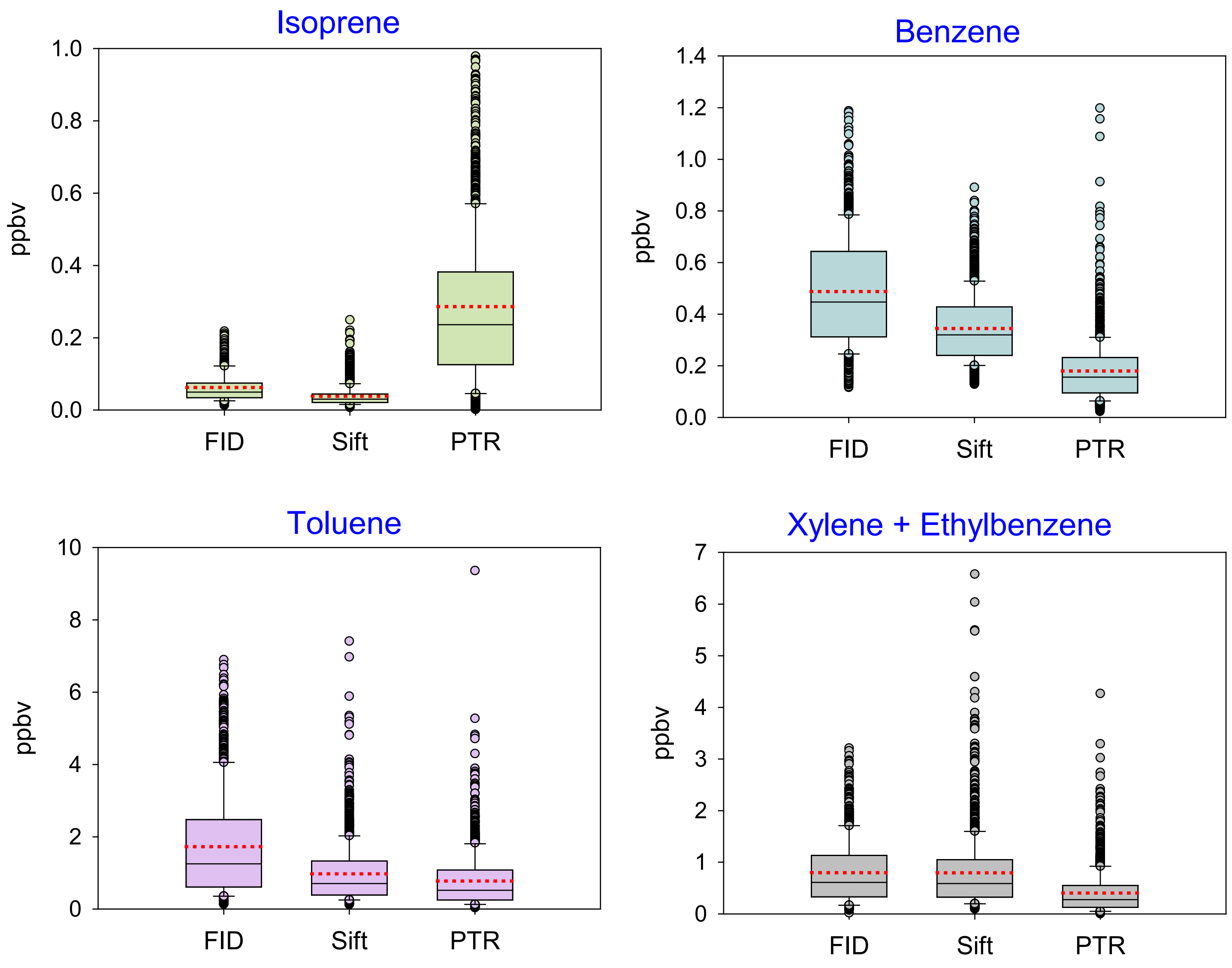
Compounds
Methanol
Acetonitrile
Acetaldehyde
Acetone, Propanal
Isoprene
MVK, Macr
MEK,Butanal
Benzene
Toluene
Styrene
C8 aromatics (ethylbenzene, m-xylene, p-xylene, and o-xylene)
Chlorobenzene
C9 aromatics
Monoterpenes
Dichlorobenzene
Trichlorobenzene

Sift-MS (possible library)

1-nitropropane	ethene, ethane
1.1.1-trichloroethane	formaldehyde
1.2-dichloroethane	formic acid
1.2-dichloropropane	Freon 113
1.2.3-trimethylbenzene	hexane
1.2.4-trichlorobenzene	hydrogen sulfide
1.3-butadiene	isobutyl alcohol
2-butene (cis, trans)	isoprene, furan
2-chloroethyl ether	menthol
2-chlorotoluene	methanol
2-methylaziridine	methyl acetate
2-pentene (cis, trans)	methyl bromide
2.5-dimethylfuran, furfural	methyl chloride
acetaldehyde	methyl iodide
acetic acid	methyl vinyl ketone, methacrolein
acetone	n-nitrosomorpholine
acetonitrile	n,n-dimethylaniline
acetylene	n,n-dimethylformamide
acrolein	naphthalene
acrylamide	cresol
acrylic acid, butanone	pentane
alpha-pinene	pentanoic acid
ammonia	perfluorotoluene
aniline	phenol, dimethyl disulfide
benzaldehyde	propane
benzene	propanoic acid
benzonitrile	propene
butane	propyne
butanoic acid, ethyl acetate	styrene
carbon disulfide	tetrachloroethylene
carbon tetrachloride	tetradecane
carbonyl sulfide	toluene
chlorobenzene	trichloroethylene
chloroform	tridecane
dichlorodifluoromethane	triethylamine
dimethyl sulfide	urethane
dodecane	vinyl acetate
ethanedial	xylenes, ethylbenzene

Inter-comparison

Online TD-GC-FID / PTR-MS / Sift-MS



Round robin test

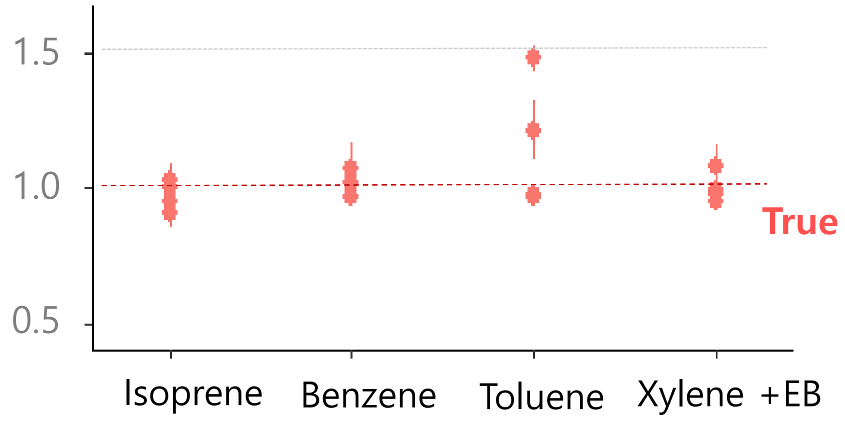
Certified low concentration STD

Test Instruments : Online TD-GC-FID

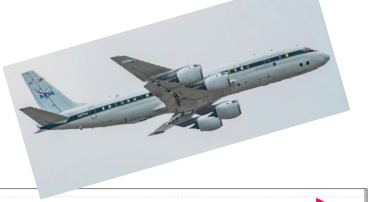
Online PTR-MS

Offline TD-GC-MS

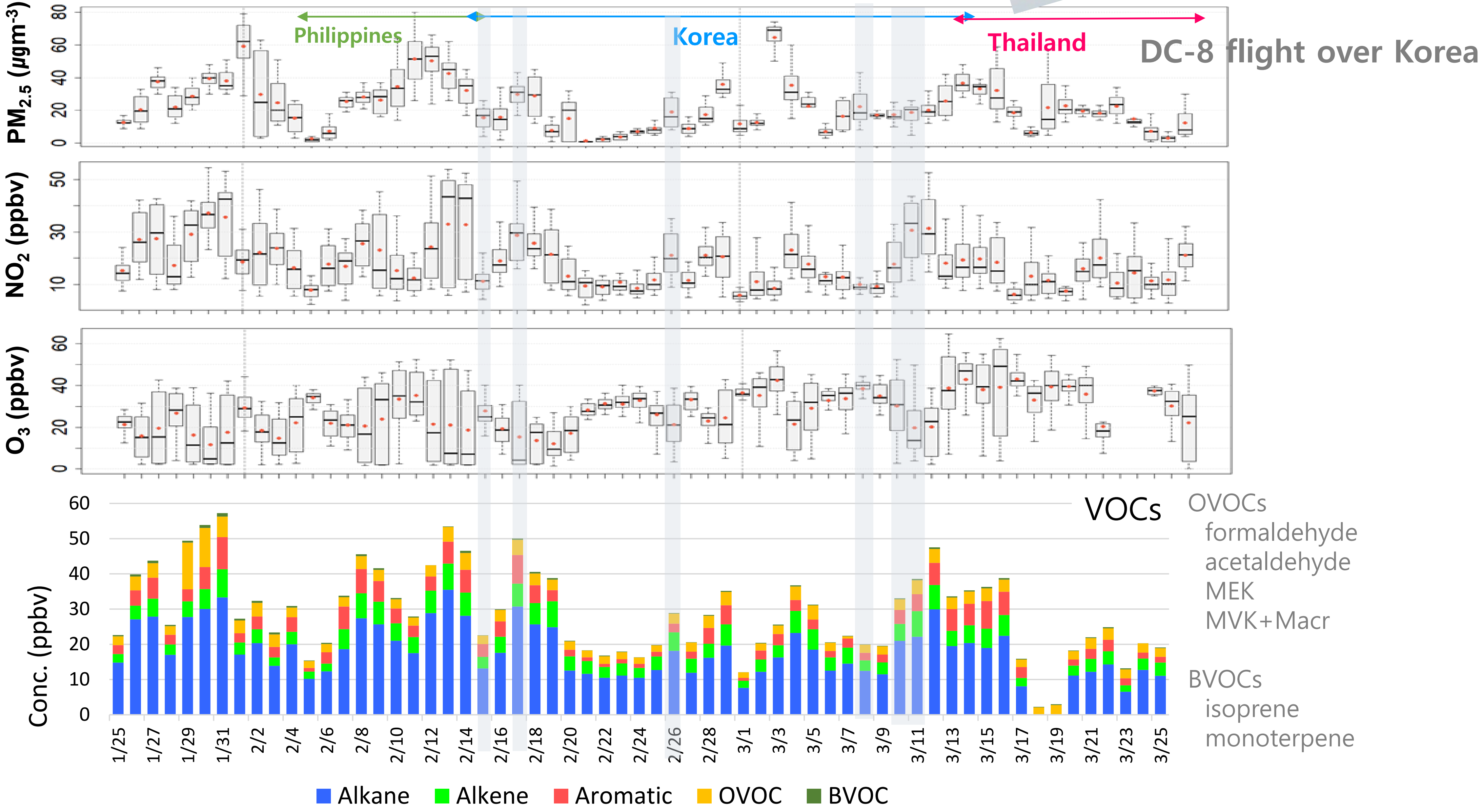
True ± 2% ~ 10% variations



Temporal distribution



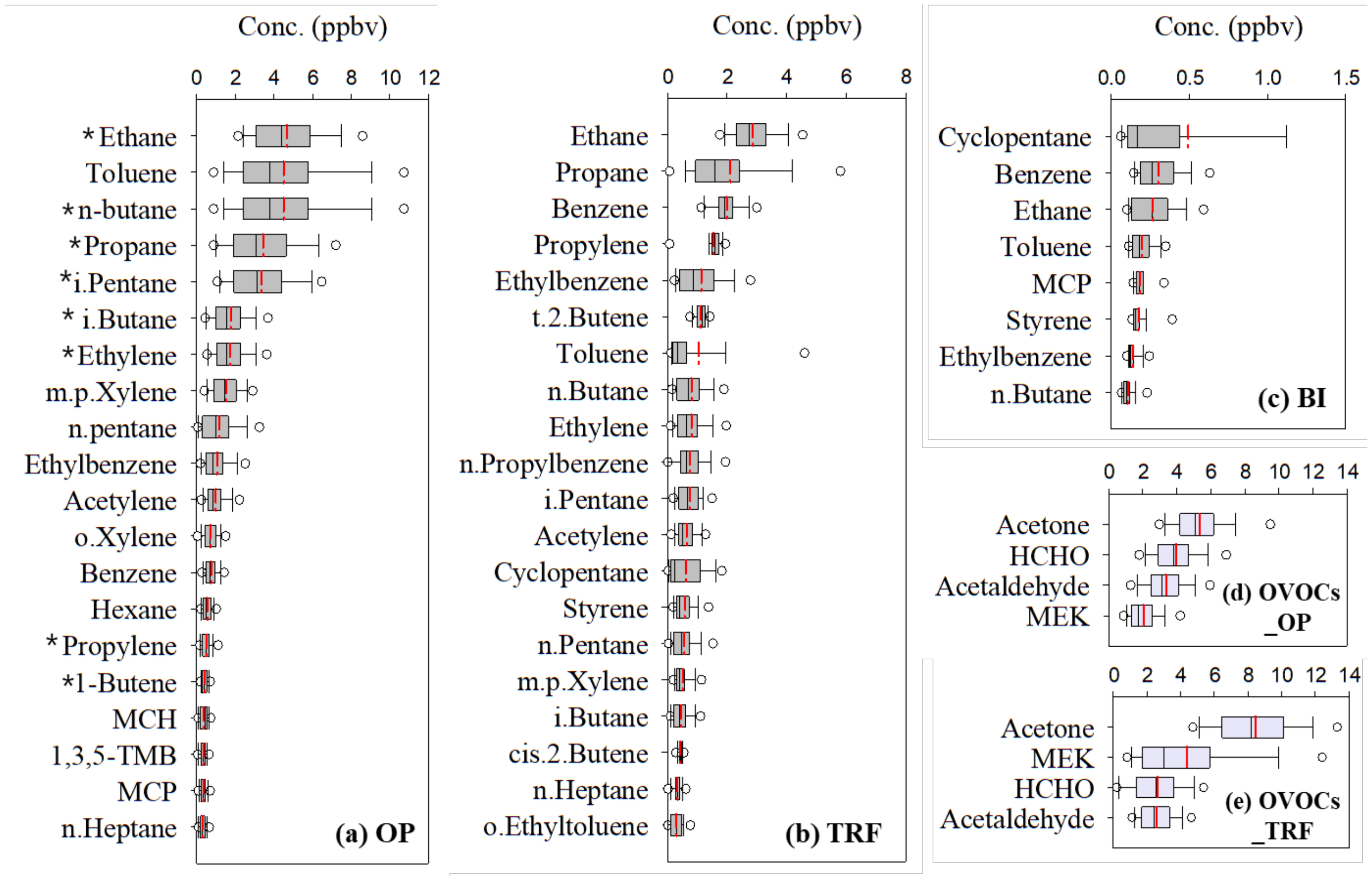
ASIA-AQ campaign

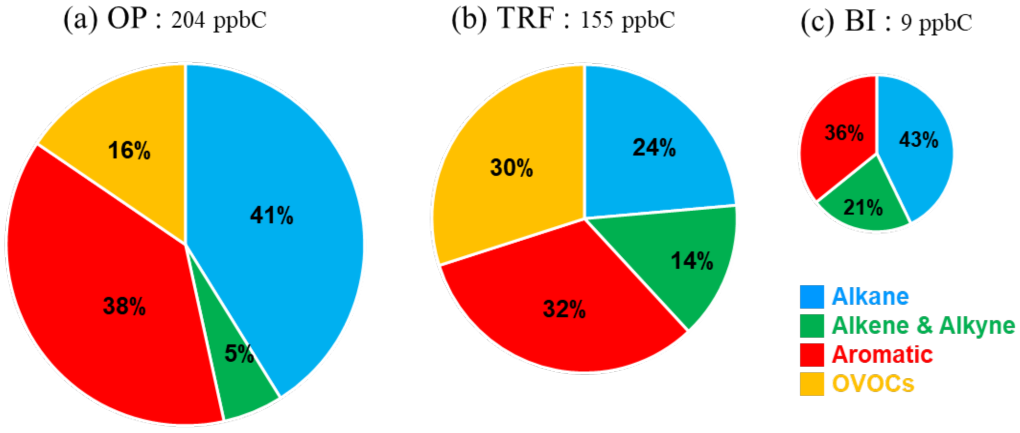


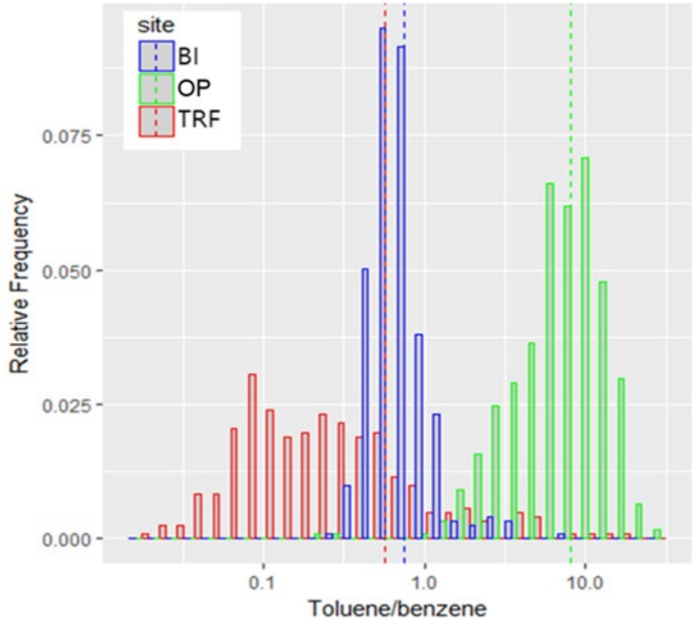
Concentrations

Abundance 1st–20th Species	Mean (ppbv)	Median (ppbv)	Max	95%ile	Detection rate
Ethane	6.84±4.13	5.47	23.26	15.66	97%
Propane	5.47±3.61	4.46	19.48	13.27	97%
Acetone	3.00±2.62	2.10	21.68	8.23	100%
Formaldehyde	2.56±2.59	2.41	39.00	5.55	100%
Ethylene	2.23±1.54	1.82	7.99	13.12	97%
Acetaldehyde	2.03±1.53	1.71	14.99	5.60	100%
Toluene	1.68±1.46	1.19	6.89	3.85	98%
n-Butane	1.34±1.03	1.02	5.66	9.77	97%
Acetylene	1.13±0.74	0.95	4.21	8.92	97%
n-Hexane	0.89±0.92	0.56	5.01	4.86	96%
i-Butane	0.83±0.64	0.63	3.58	11.00	98%
i-Pentane	0.69±0.53	0.52	2.72	6.82	97%
Propylene	0.57±0.36	0.49	1.90	11.93	96%
n-Pentane	0.48±0.40	0.39	1.93	6.55	97%
Benzene	0.48±0.21	0.44	1.19	4.56	99%
Ethylbenzene	0.37±0.32	0.27	1.71	3.53	97%
m/p-Xylene	0.36±0.30	0.27	1.50	3.45	97%
MEK	0.35±0.35	0.22	2.76	6.03	100%
Styrene	0.35±0.28	0.26	1.44	3.37	97%
Cyclopentane	0.25±0.23	0.19	1.28	7.11	98%
ΣAlkanes	18.6±10.4	15.77	10.37	5.46	97%
ΣAlkenes	4.47±2.47	3.86	2.47	6.02	97%
ΣAromatics	3.75±2.56	3.06	2.56	6.40	97%

Concentrations of KORUS-AQ campaign

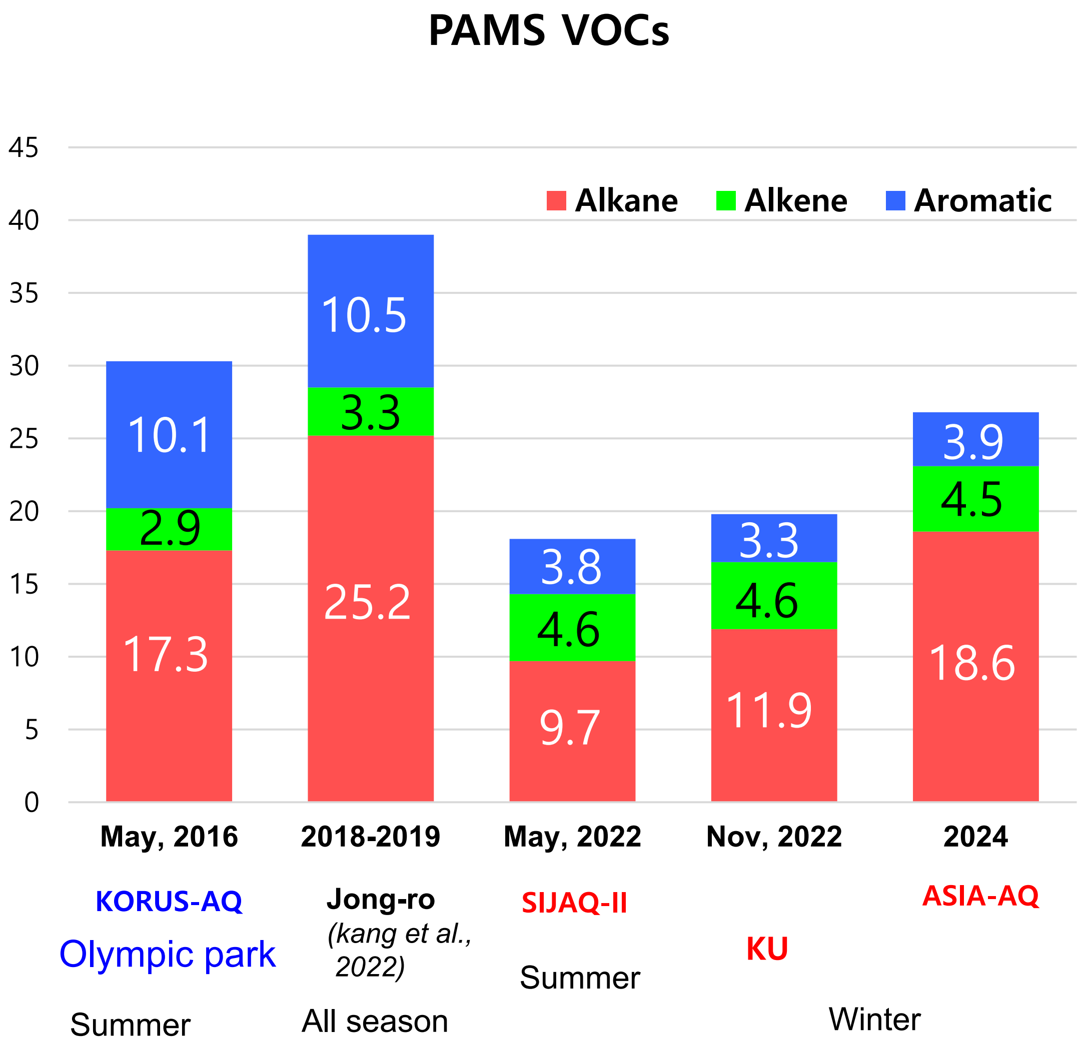


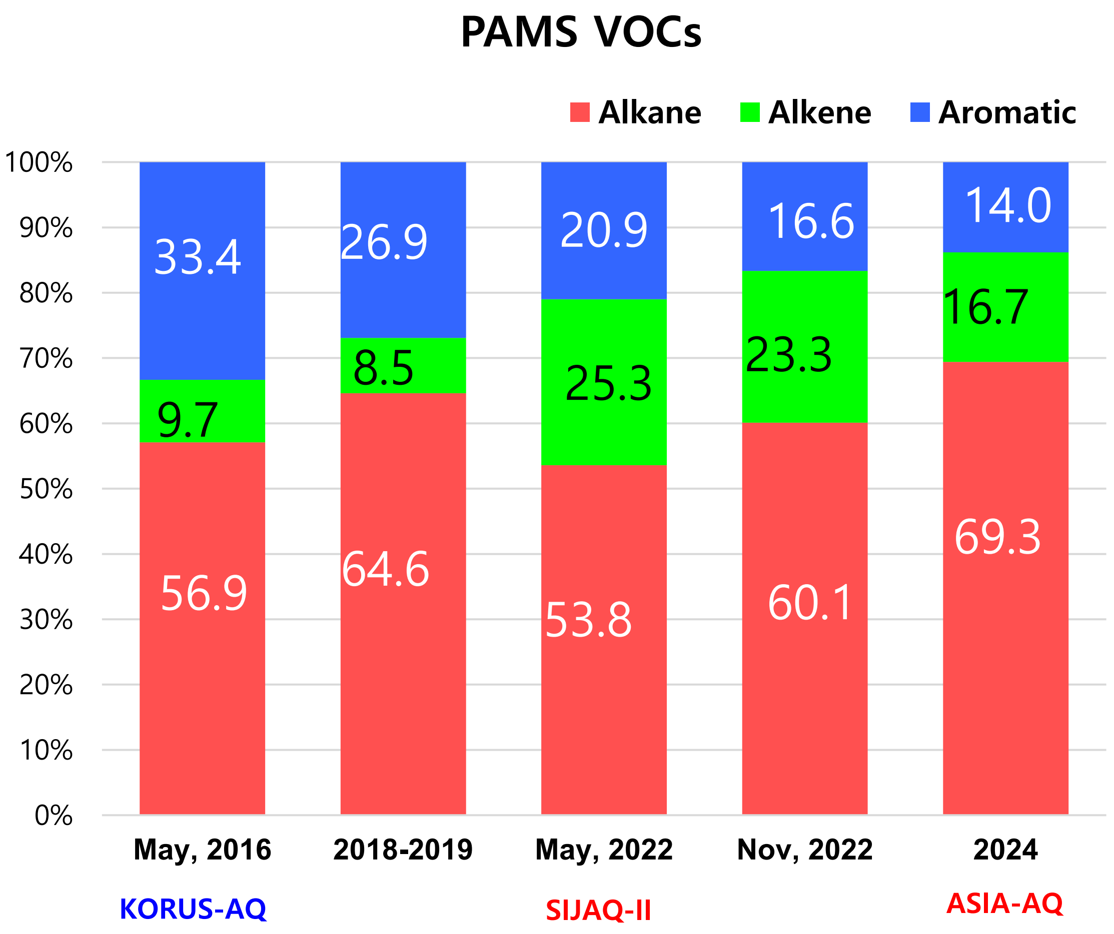




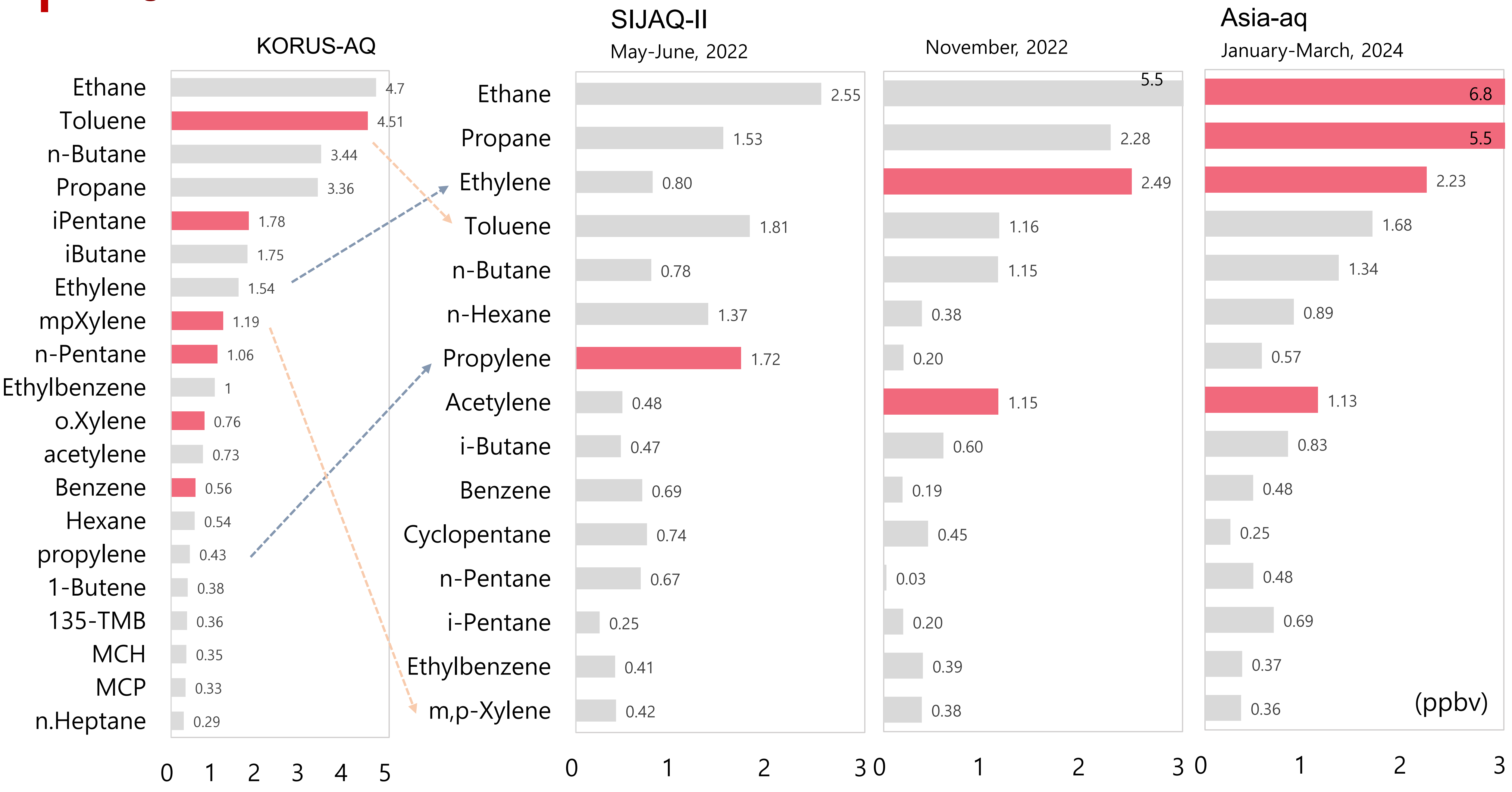
Kim et al., 2024, under review, Atmospheric Environment

Changes of VOCs

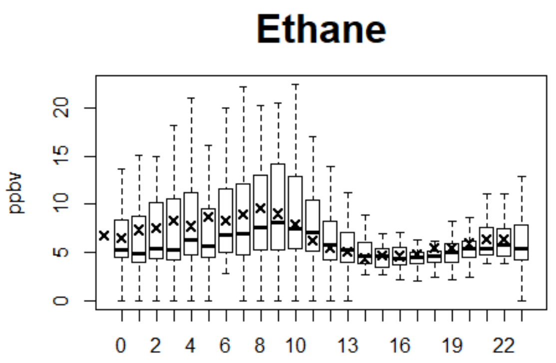


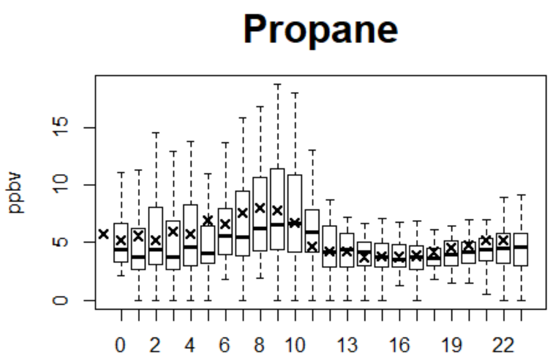


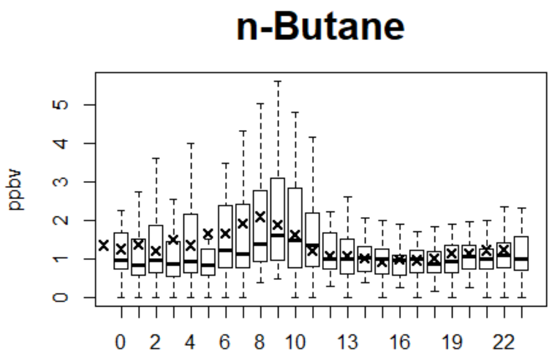
Changes of VOCs

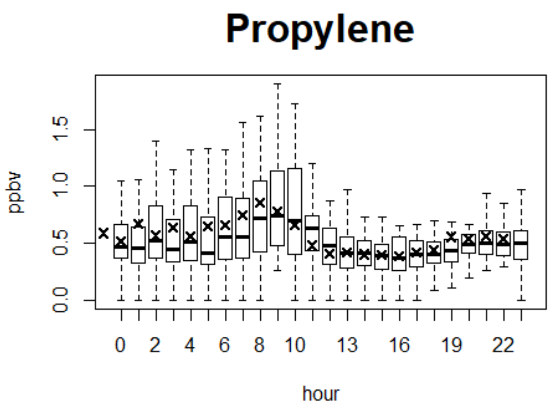


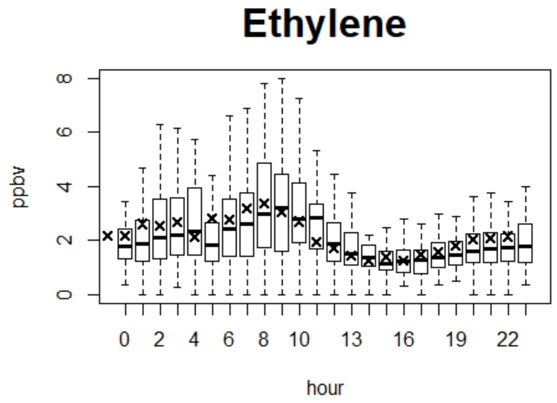
Diurnal variation, ASIA-AQ

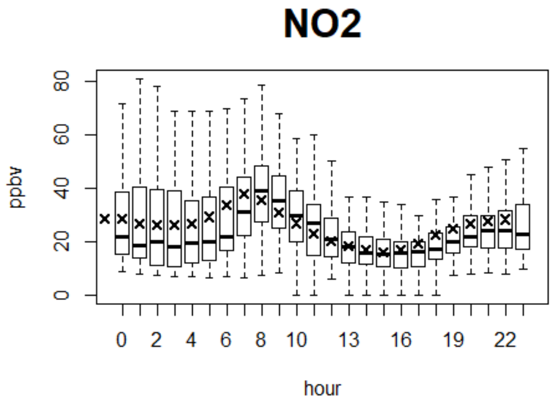


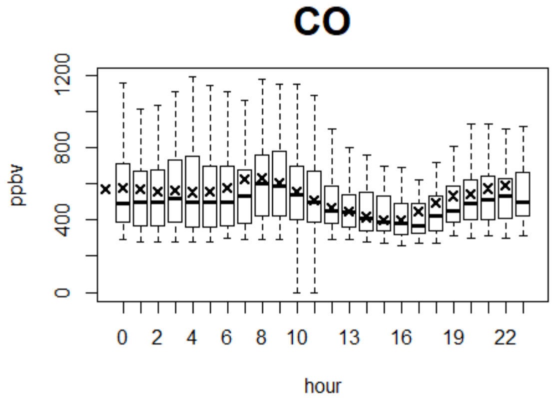


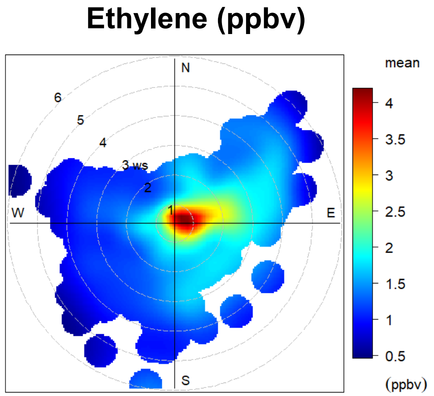


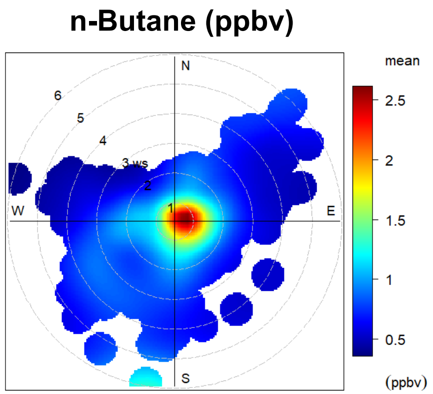


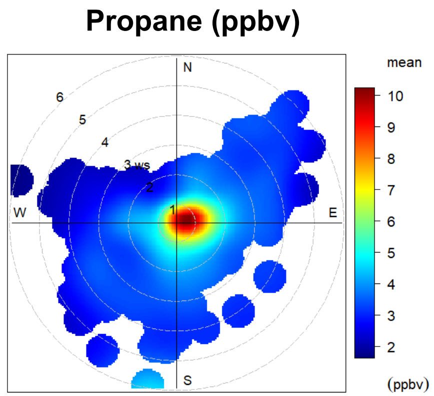


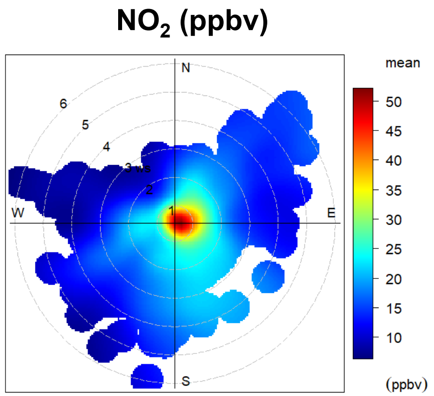






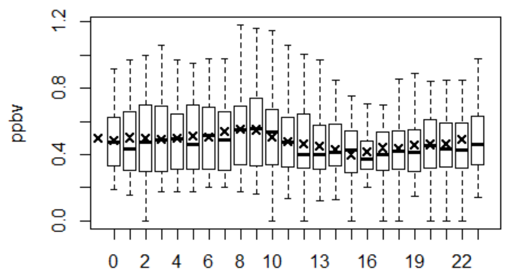




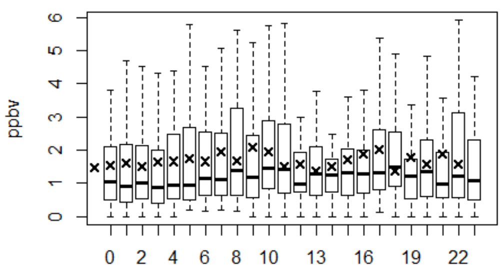


Diurnal variation, ASIA-AQ

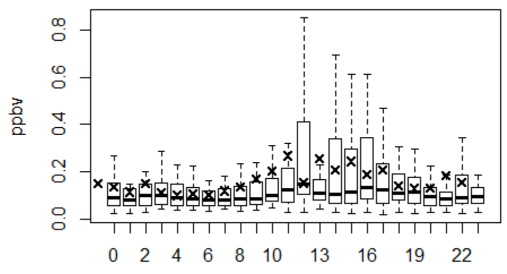
Benzene



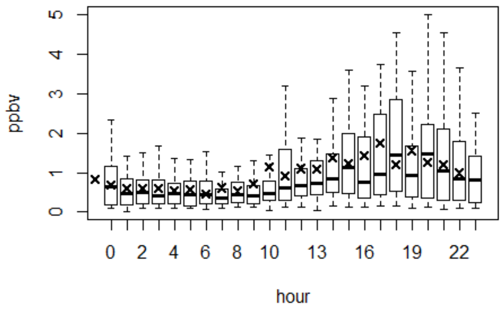
Toluene



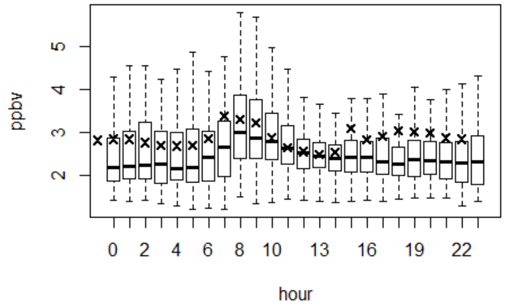
cis-2-Butene



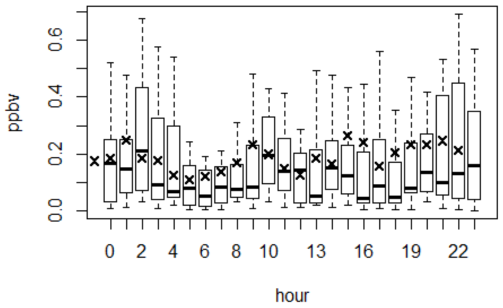
n-Hexane



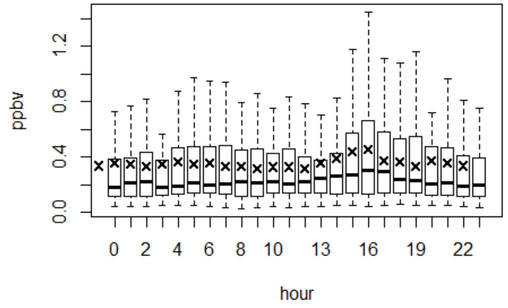
Formaldehyde



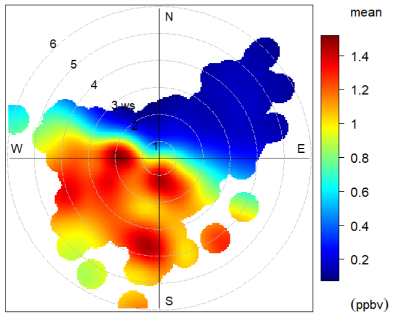
Acetaldehyde



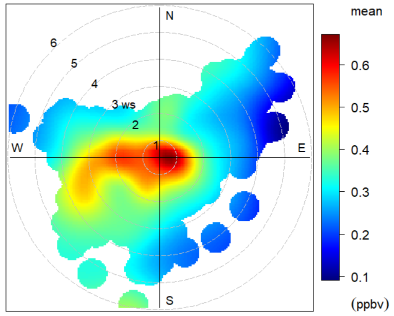
MEK



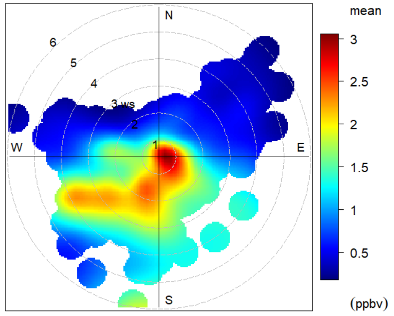
n-Hexane (ppbv)



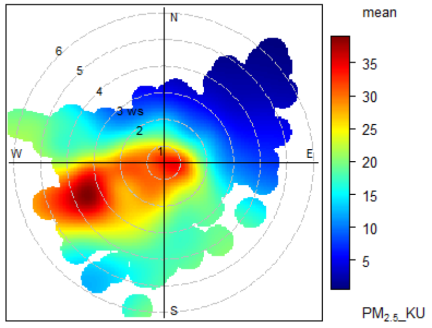
Benzene (ppbv)



Toluene (ppbv)

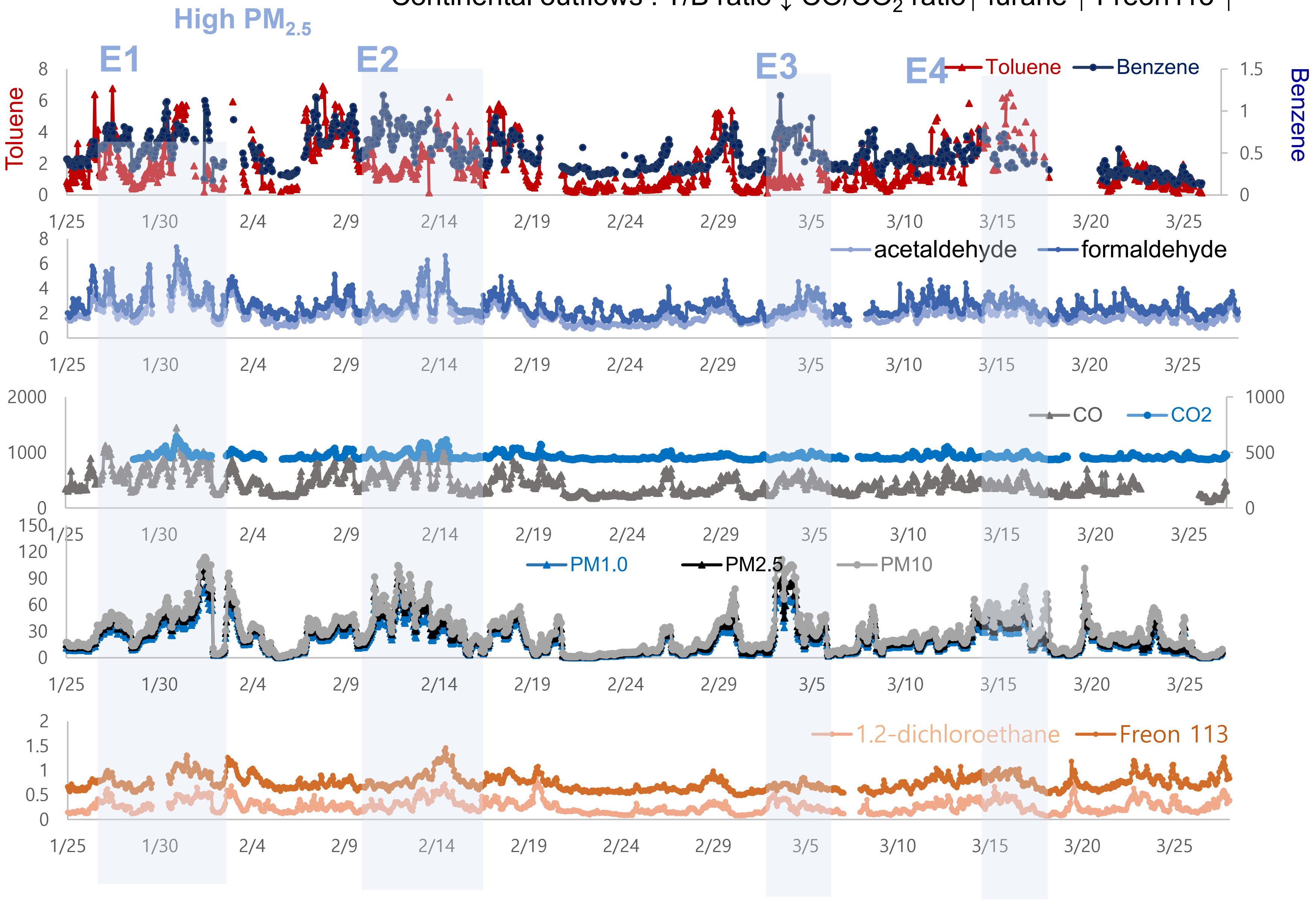


$PM_{2.5}$ (μgm^{-3})



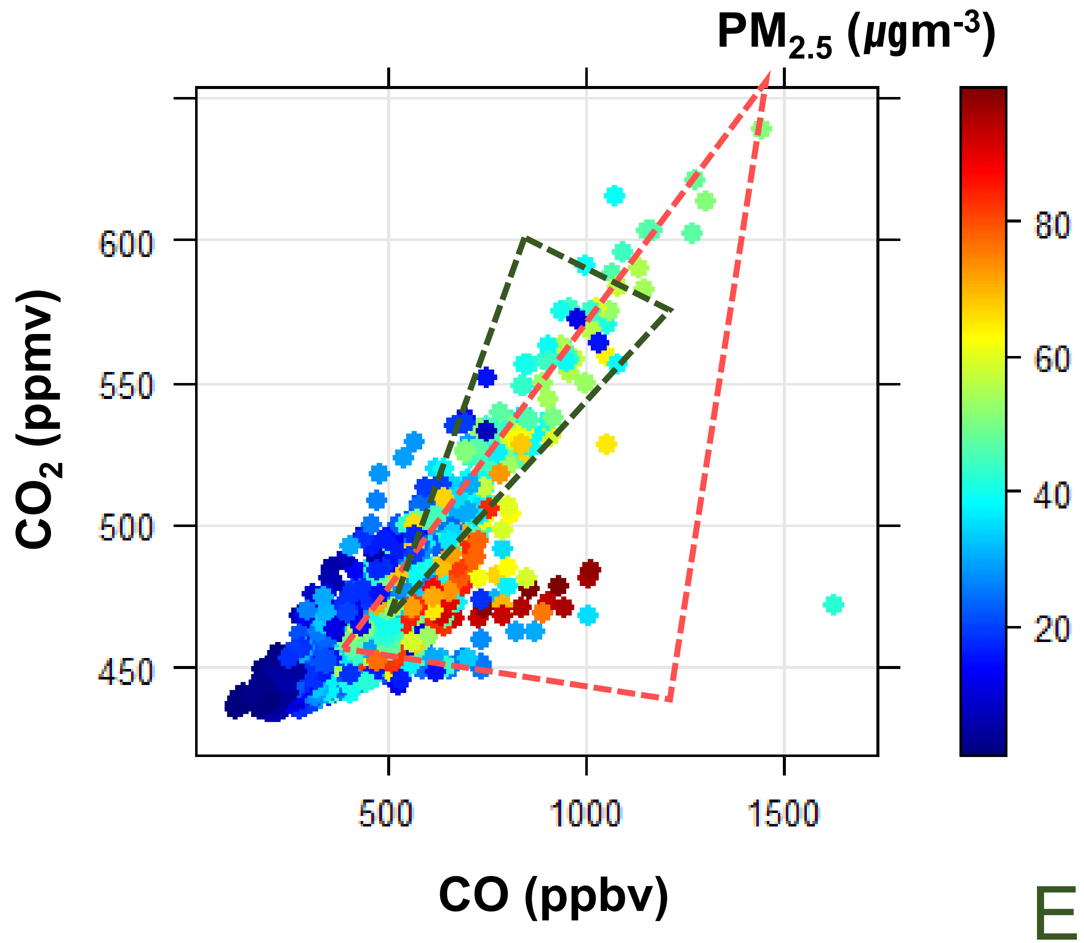
VOCs as indicators

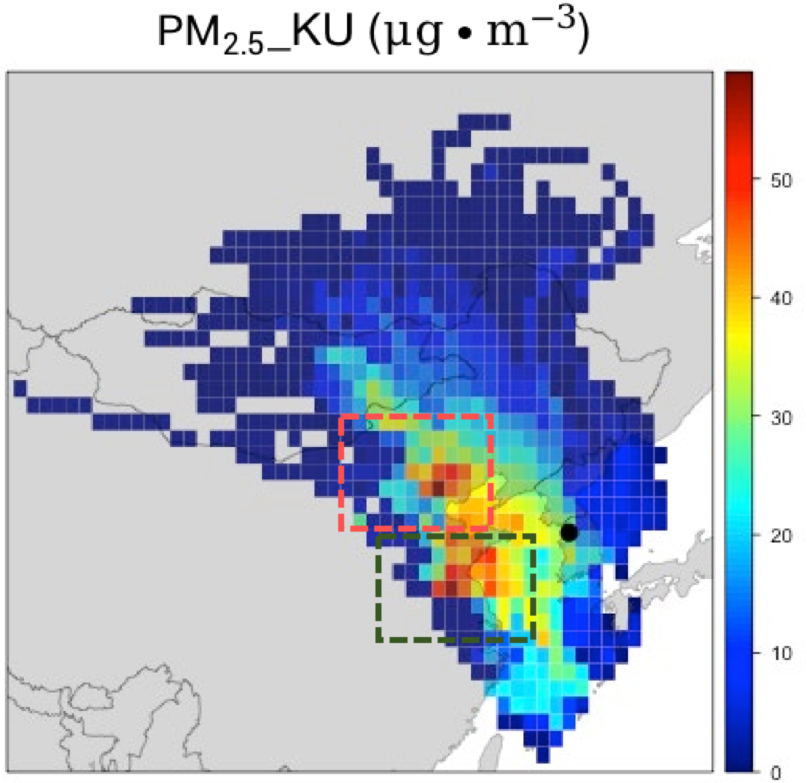
Continental outflows : T/B ratio ↓ CO/CO_2 ratio↑ furane ↑ Freon113 ↑



VOCs as indicators with high $PM_{2.5}$

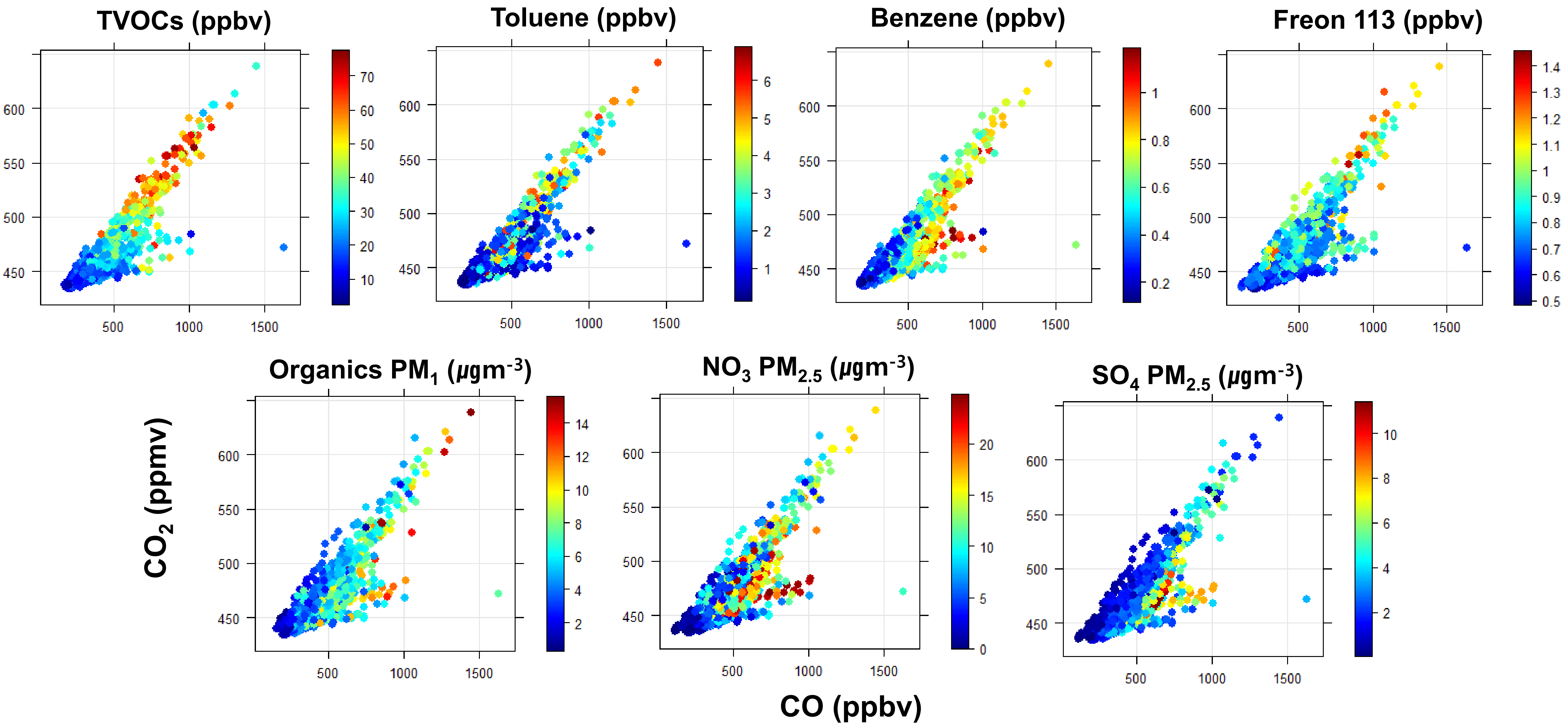
E1 & E2





E3 & E4

VOCs as indicators



Thank You

Update on ASIA-AQ in Thailand

18 May 2024

Thailand Official Committee/ Team

- The ASIA-AQ committee has officially committed to addressing air quality issues.
- Air quality researchers from both academic and government sectors across Thailand are now collaborating. We are currently gathering data from satellite sources, including burn areas, land use, and agricultural activities, along with data from ground stations.
- The most critical question for Thailand is identifying the primary and secondary sources of air pollution.
- For more information, please refer to this (https://drive.google.com/drive/folders/1y7Kvg1CqkyCmGqdnpqVkF97xvNUDeDll?usp=sharing).