

Air quality modeling of NMVOCs

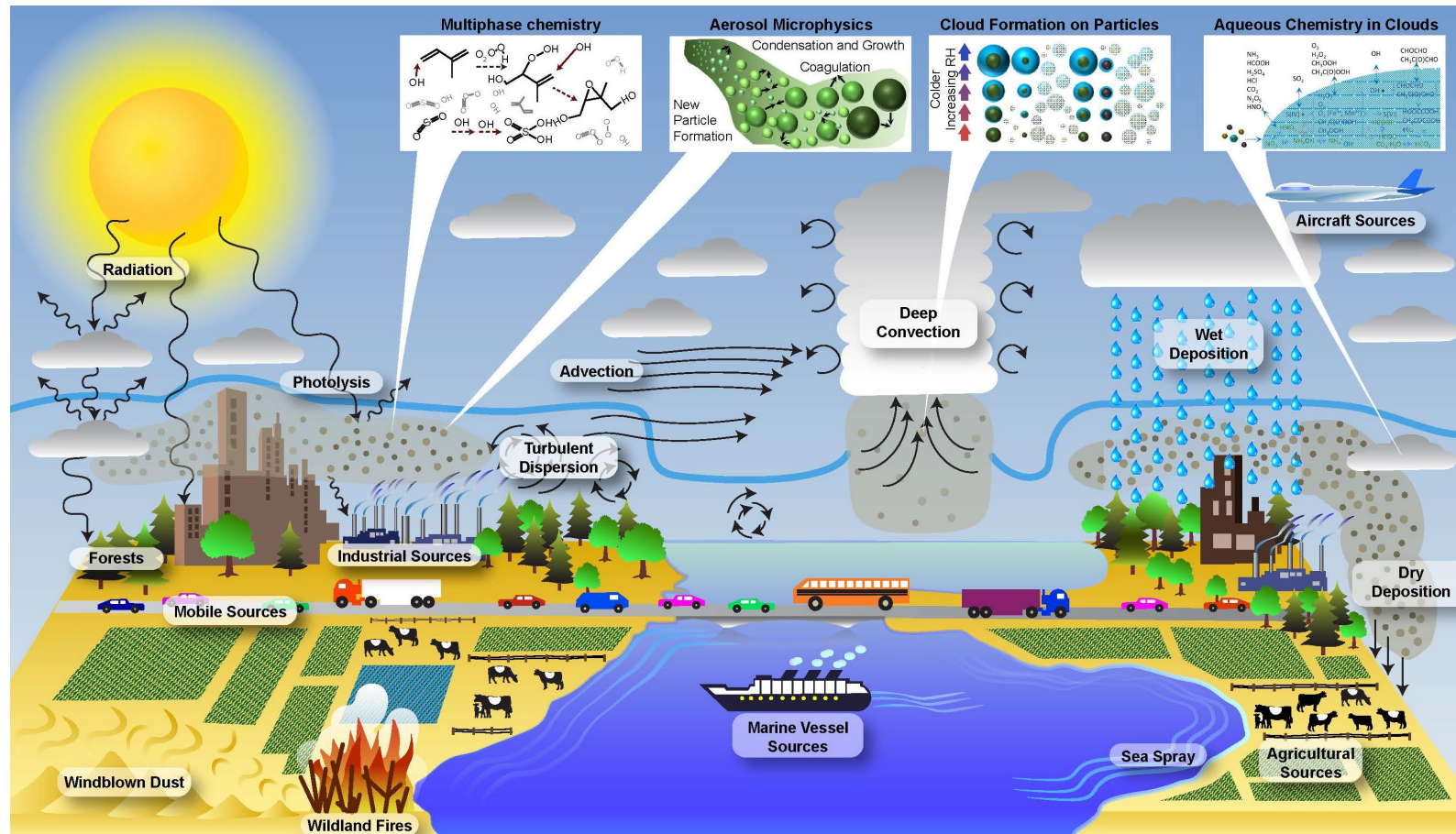
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National Institute for Environmental Studies (NIES)

Webinar Workshop for Emission Inventory of VOCs
and Its Application for Policy Consideration
December 4th, 2024

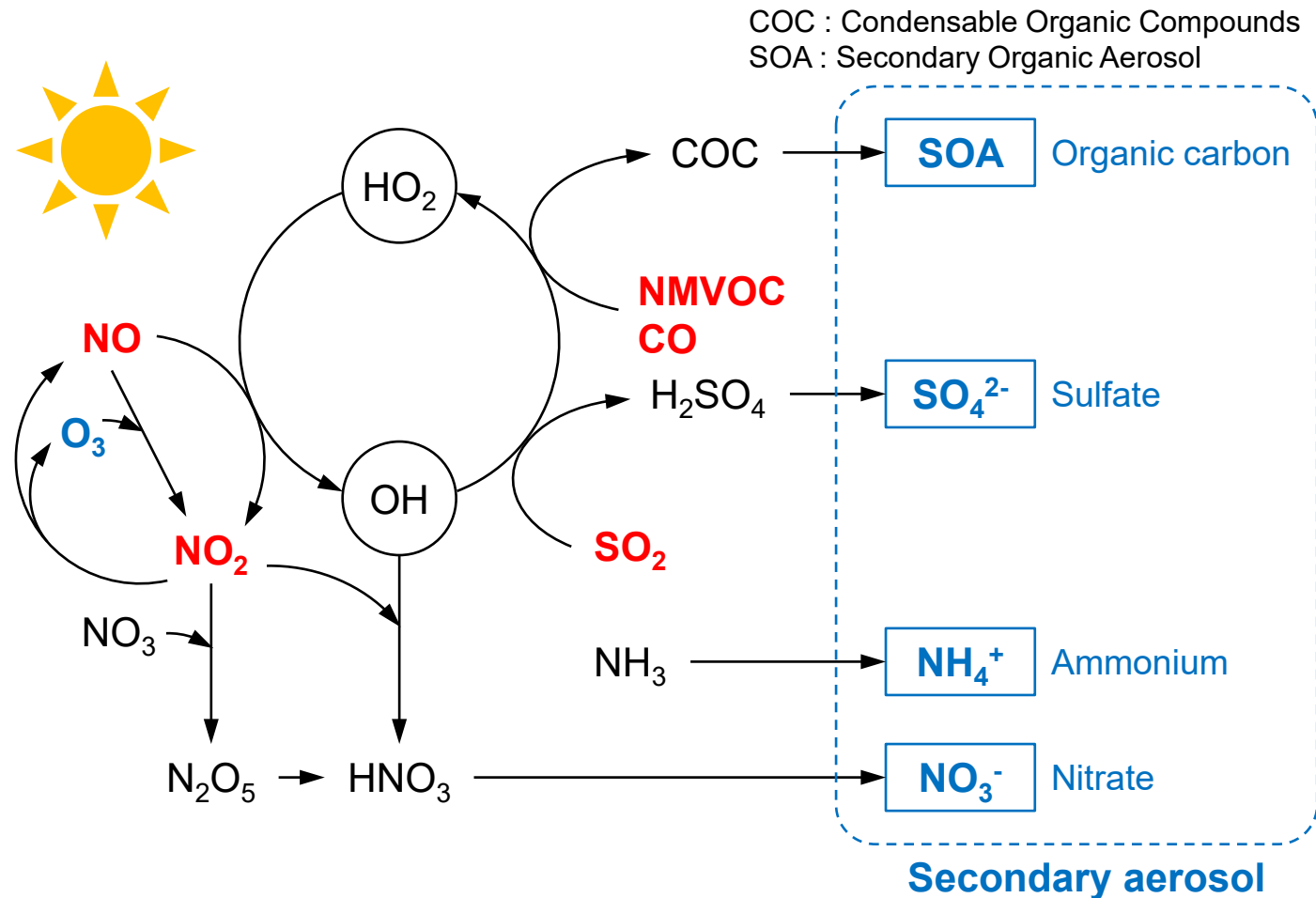
Physical and chemical processes in the atmosphere

- Ambient pollutants emitted from sources are affected by various physical and chemical processes before removed from the atmosphere.



Photochemical reaction cycle

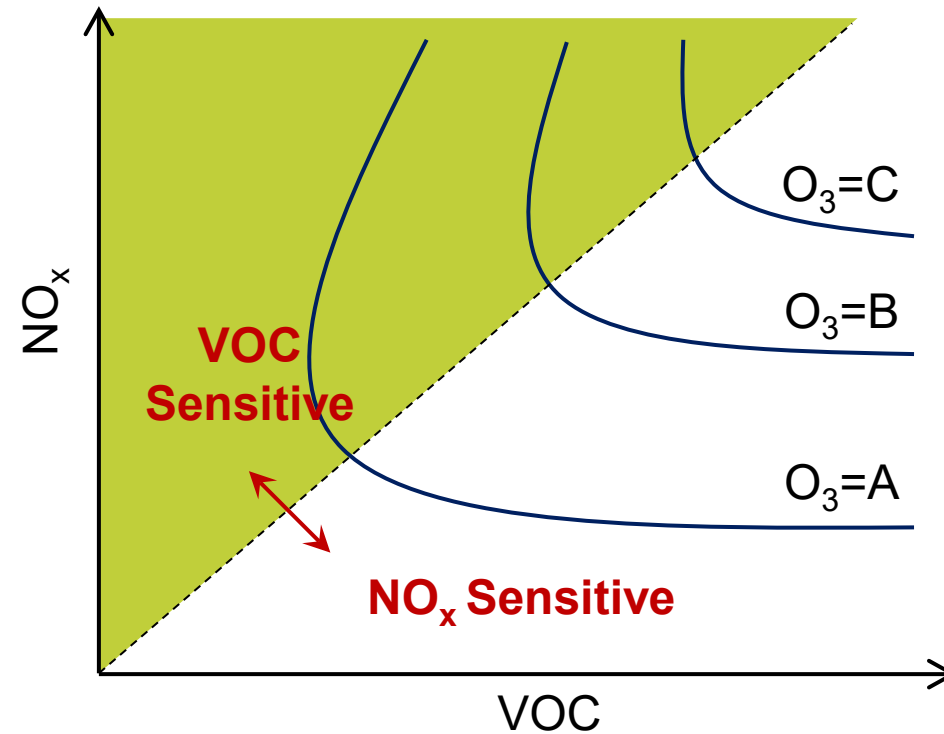
- Secondary pollutants are formed via complex photochemical reaction cycle.
- VOCs are important precursors for ozone and SOA.



(Meng et al., 1997)

Non-linear relationships

- Non-linear relationships between secondary pollutants and precursors caused by complex photochemical reaction cycle should be understood to develop effective strategies.

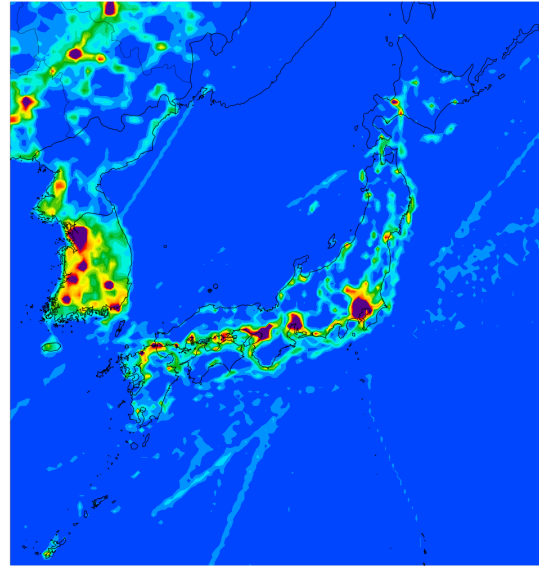


Relationship among NO_x , VOC, and ozone

3-D regional air quality simulation

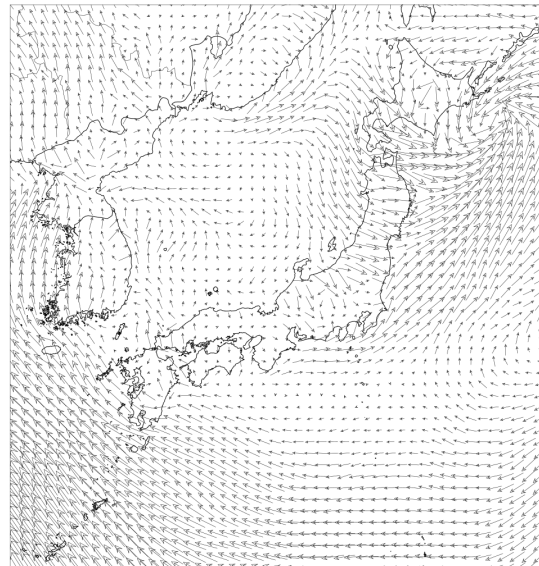
Emission inventory

Precursor emissions
from sources
with spatial and
temporal variations



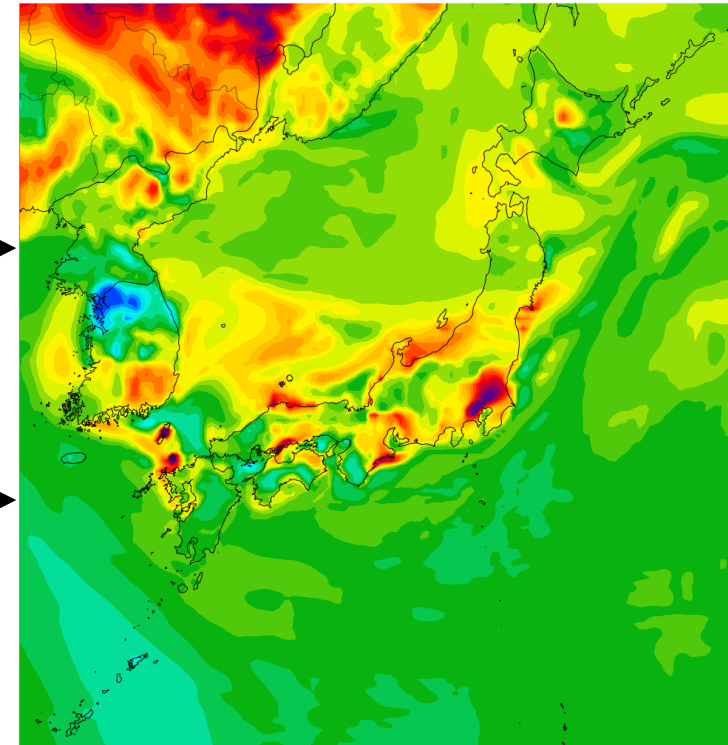
Regional Meteorological model

Simulate spatial
and temporal variations
of meteorological fields



Regional chemical transport model

Simulate spatial and
temporal variations
of ambient pollutants



Roles of air quality simulations

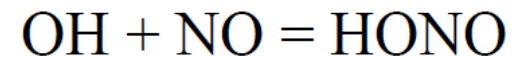
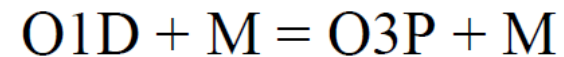
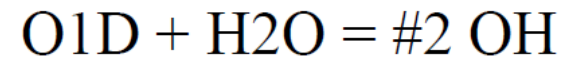
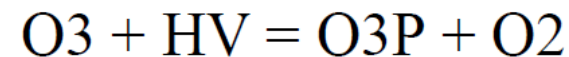
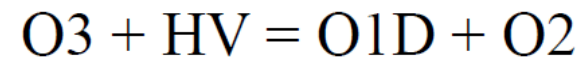
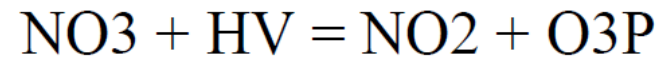
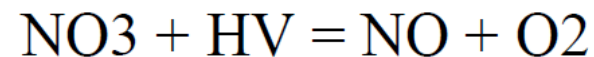
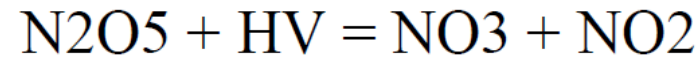
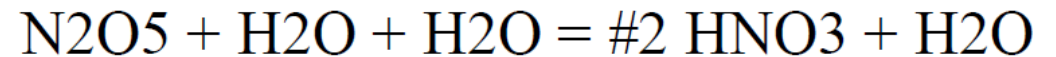
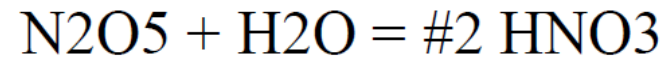
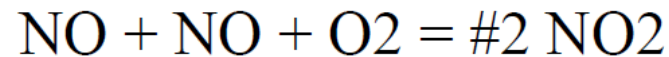
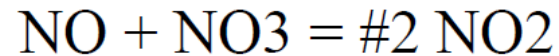
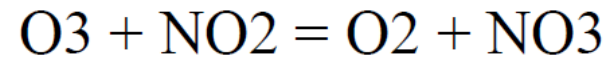
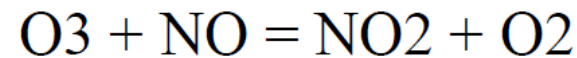
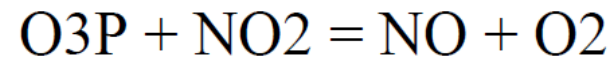
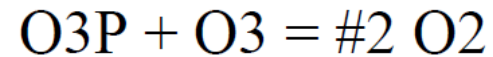
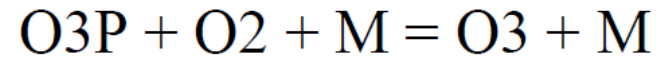
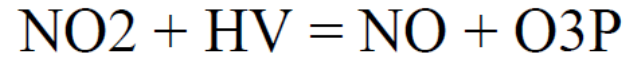
- ❑ Clarify formation mechanism of air pollution
- ❑ Identify key emission sources on ambient pollutant concentrations
- ❑ Evaluate effectiveness of emission controls implemented to suppress ambient pollutant concentrations.
- ❑ Predict ambient pollutant concentrations based on future scenarios considering various pathways of emission controls and activities
- ❑ Forecast ambient pollutant concentrations for a few coming days



- ❑ Governments utilize air quality simulations to tackle air quality issues

Photochemical reactions in models

- Important species and reactions are explicitly represented.

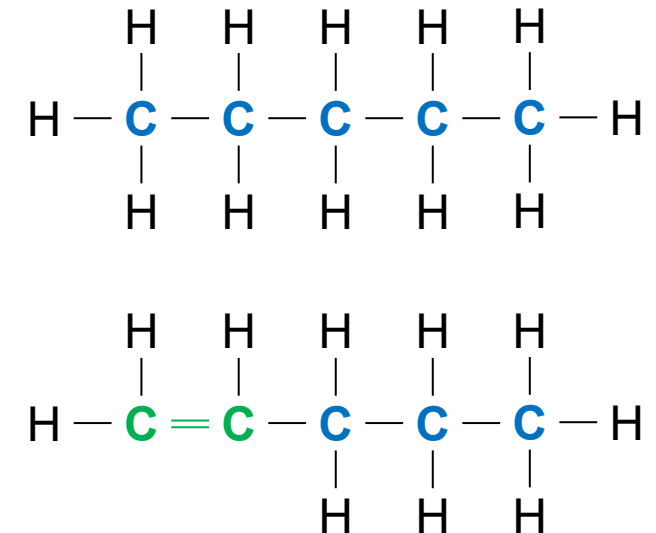


VOC representations in models

- Many kinds of VOCs exist in the atmosphere.
- Impossible to explicitly represent all individual VOCs in models.

□ Chemical mechanisms

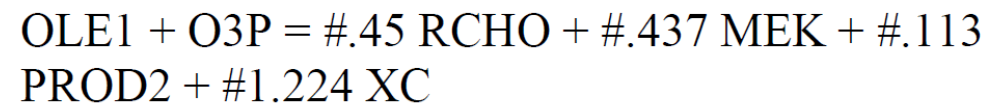
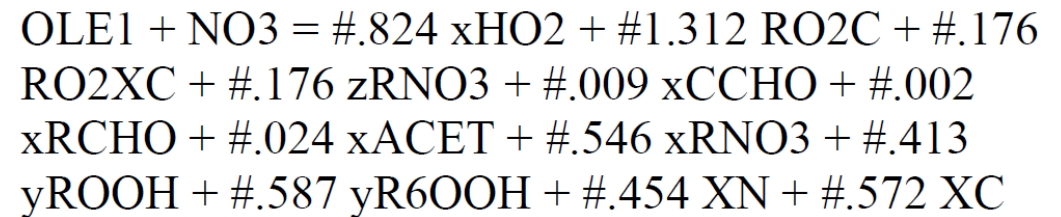
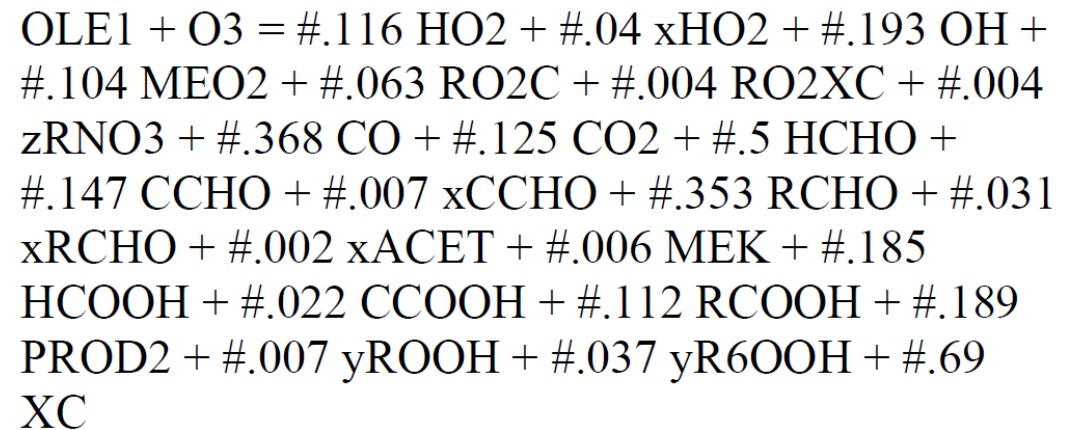
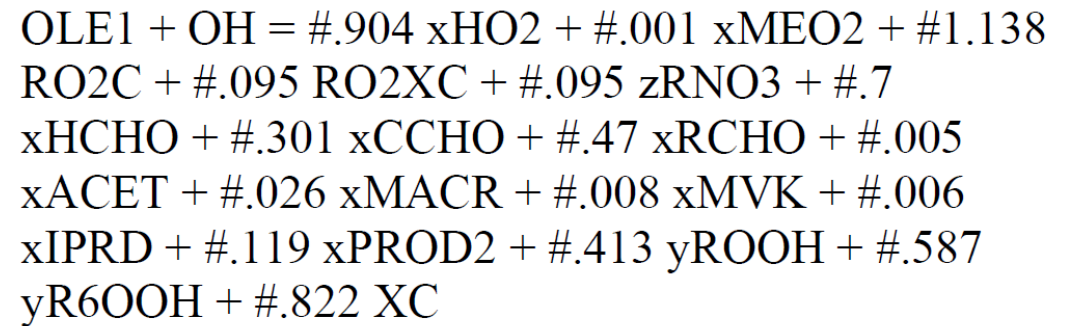
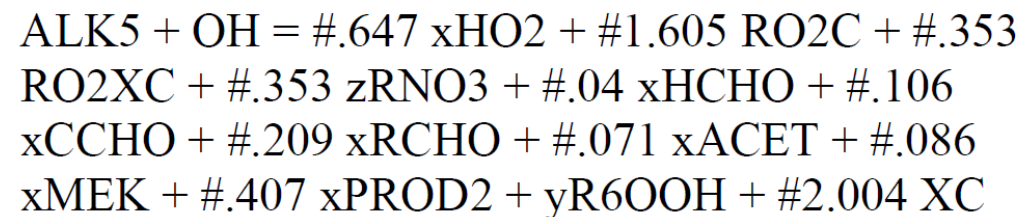
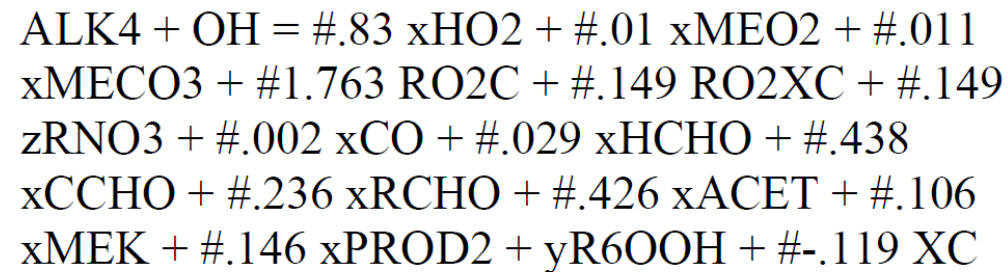
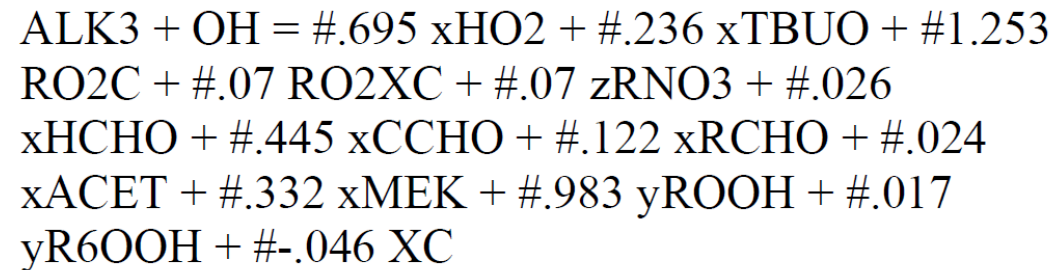
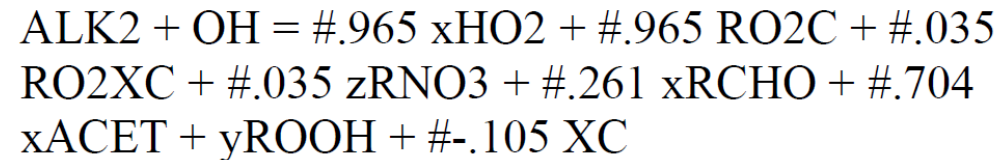
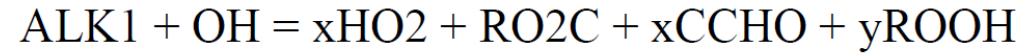
- Lump similar VOCs
- Lumping based on structures (CB6)
 - Pentane (C_5H_{12}) → 5PAR
 - 1-Pentene (C_5H_{10}) → 3PAR+1OLE
- Lumping based on reactivities (SAPRC, CRACMM)
 - Pentane (C_5H_{12}), Hexane (C_6H_{14}), Heptane (C_7H_{16}) → ALK4
- Explicitly represent important VOCs (Benzene, Toluene, Xylene, etc.)



Examples of lumped VOC species (SAPRC07)

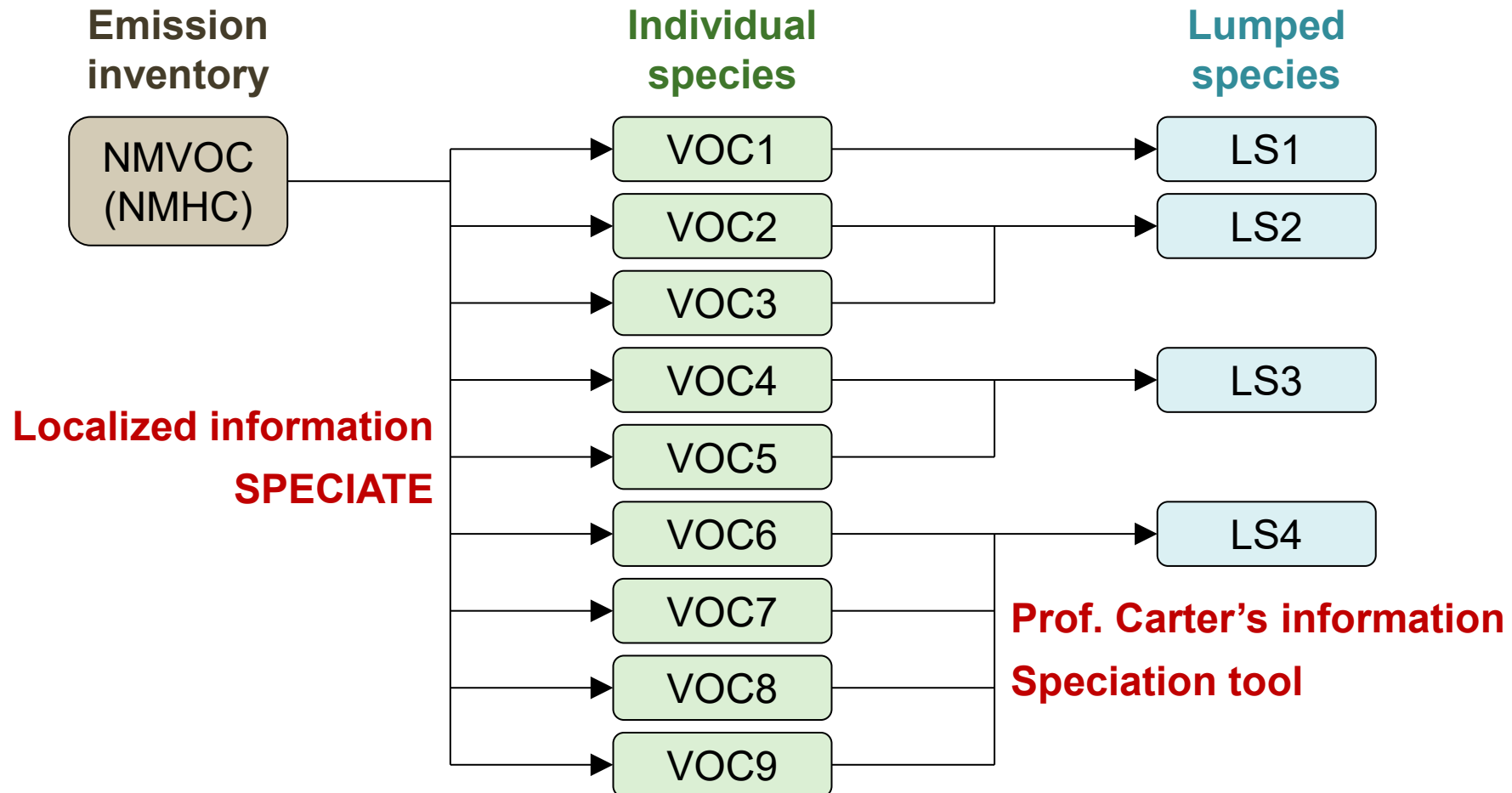
Name	Definition	Examples
ALK1	Alkanes and other non-aromatic compounds that react only with OH, and have kOH between $2 \text{ and } 5 \times 10^2 \text{ ppm}^{-1} \text{ min}^{-1}$	Ethane
ALK2	Alkanes and other non-aromatic compounds that react only with OH, and have kOH between $5 \times 10^2 \text{ and } 2.5 \times 10^3 \text{ ppm}^{-1} \text{ min}^{-1}$	Propane
ALK3	Alkanes and other non-aromatic compounds that react only with OH, and have kOH between $2.5 \times 10^3 \text{ and } 5 \times 10^3 \text{ ppm}^{-1} \text{ min}^{-1}$	Butane
ALK4	Alkanes and other non-aromatic compounds that react only with OH, and have kOH between $5 \times 10^3 \text{ and } 1 \times 10^4 \text{ ppm}^{-1} \text{ min}^{-1}$	Pentane, Hexane, Heptane
ALK5	Alkanes and other non-aromatic compounds that react only with OH, and have kOH greater than $1 \times 10^4 \text{ ppm}^{-1} \text{ min}^{-1}$	Octane, Nonane, Decane
ARO1	Aromatics with kOH $< 2 \times 10^4 \text{ ppm}^{-1} \text{ min}^{-1}$	Propylbenzene
ARO2	Aromatics with kOH $> 2 \times 10^4 \text{ ppm}^{-1} \text{ min}^{-1}$	Ethyltoluene
OLE1	Alkenes (other than ethene) with kOH $< 7 \times 10^4 \text{ ppm}^{-1} \text{ min}^{-1}$	1-Butene, 1-Pentene
OLE2	Alkenes with kOH $> 7 \times 10^4 \text{ ppm}^{-1} \text{ min}^{-1}$	2-Butene, 2-Pentene

Photochemical reactions of lumped species (SAPRC07)



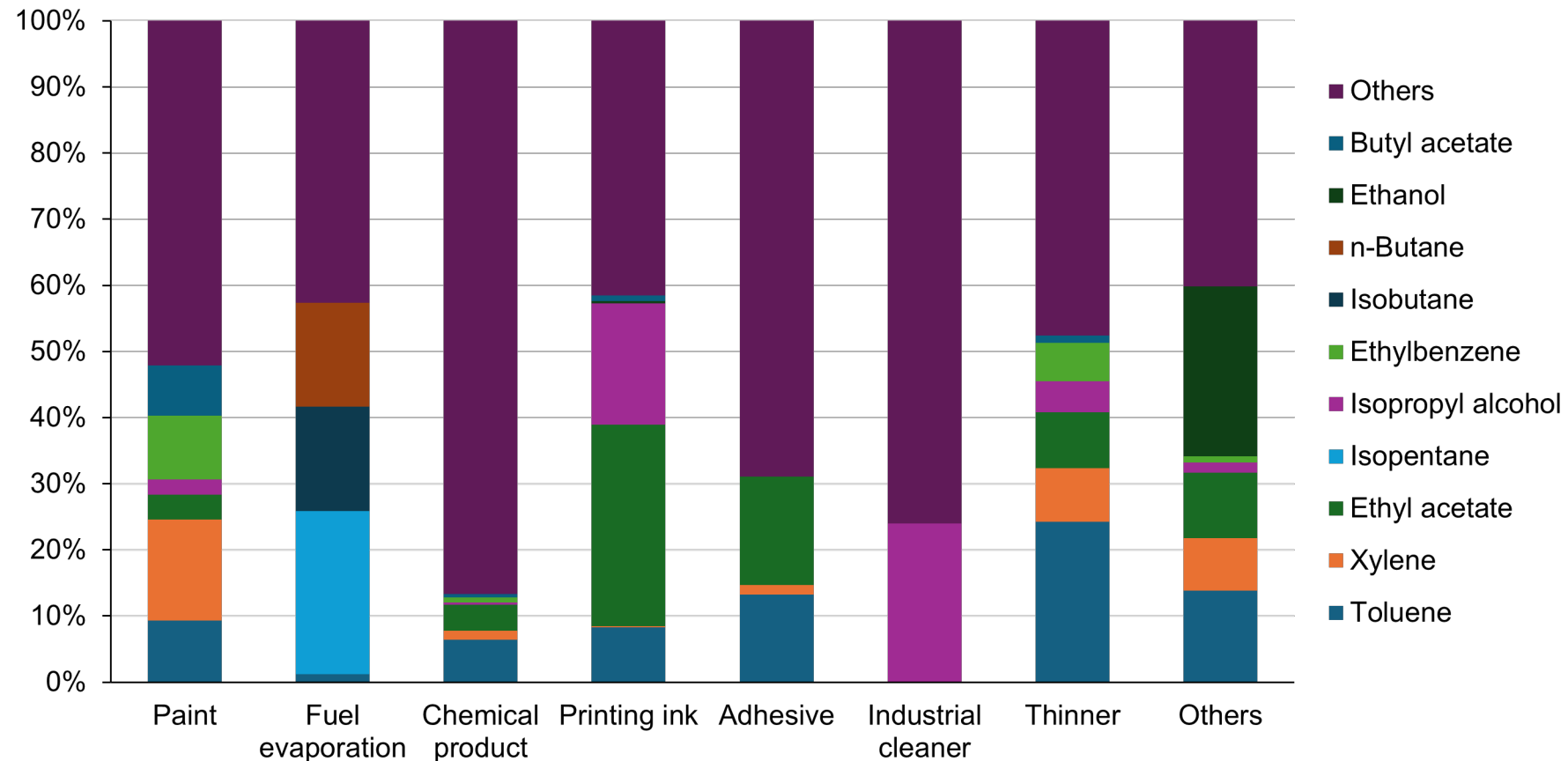
VOC speciation

- Need to speciate VOC emissions into lumped species in chemical mechanisms.



Local information of VOC profiles

- Profiles in addition to total emission amounts of VOCs are compiled in emission inventories.



VOC profiles compiled in the VOC emission inventory in Japan

SPECIATE

- VOC profiles of various emission sources are available.

<https://www.epa.gov/air-emissions-modeling/speciate>

The screenshot displays the EPA website's SPECIATE Data Browser interface. At the top, the EPA logo and navigation menu are visible. The main heading is "SPECIATE" with sub-links for Introduction, Browser, Download, Documentation, and Development. The "SPECIATE Data Browser" section explains its purpose and lists several features: Profile - Detail, Profile - Basic, Profile List, Species Properties, Weight % (bar), Weight % (pie), and Revisions. A help guide link is provided below. The main data table is titled "Profile Data - Basic" and shows the following data:

PROFILE_CODE	PROFILE_NAME	SPECIES_NAME	WEIGHT_PERCENT	PROFL...	PROFILE...	MASTE...	VERSL...	REGION
1	External Combustion Boiler - Residual Oil	Formaldehyde	42	YES	GAS	-	3.2	-
1	External Combustion Boiler - Residual Oil	Acetone	28	YES	GAS	-	3.2	-
1	External Combustion Boiler - Residual Oil	N-butane	14	YES	GAS	-	3.2	-
1	External Combustion Boiler - Residual Oil	Methane	11	YES	GAS	-	3.2	-
1	External Combustion Boiler - Residual Oil	N-hexane	5	YES	GAS	-	3.2	-

Lumping information

- Relationships between individual and lumped species are available.
 - Prof. Carter's information (<https://intra.engr.ucr.edu/~carter/emitdb/SpecDB.xls>)
 - Speciation tool (https://www.cmascenter.org/speciation_tool/)

Individual Compounds in DB

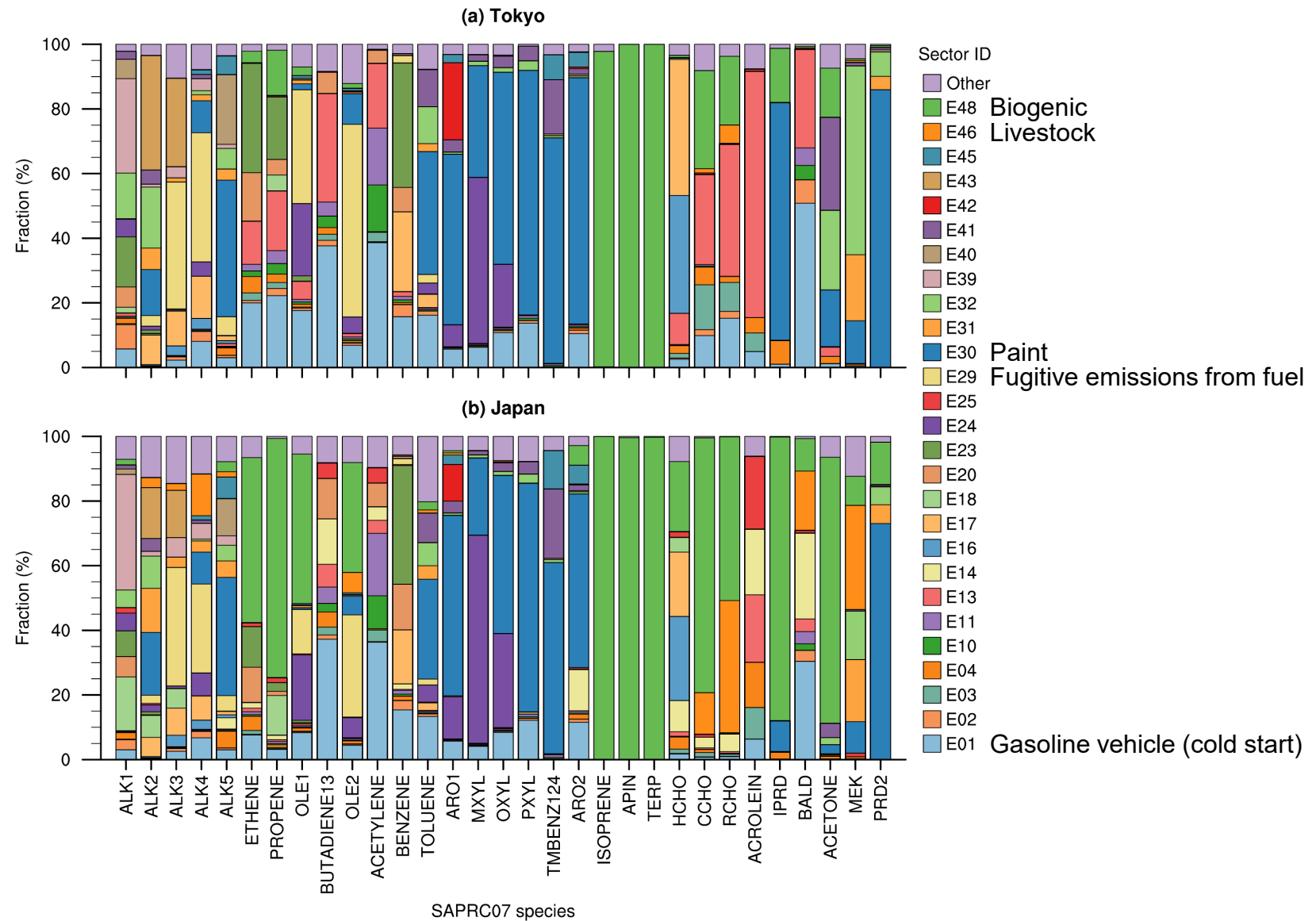
Max: 1.000 1.000 1.000 1.455 0.154 1.000 3/2/23
 No or Min: 1817 0.295 1817 0.150 1817 0.003 2 0.154 1817 0.150 1817 1817

Model species assignments for mechanisms ->

Unique ID	Description	S99	S07	S07T	C.S07	S11	S11D	S16C	S18B	S22
C2943-75-1	Triethoxyoctylsilane									
C5124-30-1	methylene-bis(4-cyclohexylisocya									
C67-54-1	acetone	ACET	1.000 ACET	1.000 ACET	1.000 PRD2	0.071	ACET	1.000 ACET	ACET	ACET
C74-86-2	acetylene	ALK2	1.000 ACYE	1.000 ACYE	1.000 ALK3	0.308	ACYL	1.000 ACYL	ACETL	ACETL
C107-13-1	acrylonitrile	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 ACRYLNIT	OTH4	OTH4
C107-02-8	acrolein (2-propenal)	MACR	1.000 MACR	1.000 ACRO	1.000 IPRD	1.000	MACR	1.000 ACRO	ACRO	ACRO
C287-92-3	cyclopentane	ALK4	1.000 ALK4	1.000 ALK4	1.000 ALK4	1.000	ALK4	1.000 CYCOS	ALK4	ALK4
C109-56-0	n-pentane	ALK4	1.000 ALK4	1.000 ALK4	1.000 ALK4	1.000	ALK4	1.000 NCS	ALK4	ALK4
C78-78-4	2-methyl-butane	ALK4	1.000 ALK4	1.000 ALK4	1.000 ALK4	1.000	ALK4	1.000 M2C4	ALK4	ALK4
C110-54-3	n-hexane	ALK4	1.000 ALK4	1.000 ALK4	1.000 ALK4	1.000	ALK4	1.000 NCS	ALK4	ALK4
C107-83-5	2-methylpentane	ALK4	1.000 ALK4	1.000 ALK4	1.000 ALK4	1.000	ALK4	1.000 M2C5	ALK4	ALK4
C96-14-0	3-methylpentane	ALK4	1.000 ALK4	1.000 ALK4	1.000 ALK4	1.000	ALK4	1.000 M3C5	ALK4	ALK4
C78-29-4	2,3-dimethylbutane	ALK4	1.000 ALK4	1.000 ALK4	1.000 ALK4	1.000	ALK4	1.000 M22C4	ALK4	ALK4
C1638-26-2	1,1-dimethylcyclopentane	ALK4	1.000 ALK4	1.000 ALK4	1.000 ALK4	1.000	ALK4	1.000 M11CC5	ALK4	ALK4
C464-06-2	2,2,3-trimethylbutane	ALK4	1.000 ALK4	1.000 ALK4	1.000 ALK4	1.000	ALK4	1.000 M223C4	ALK4	ALK4
C108-08-7	2,4-dimethylpentane	ALK4	1.000 ALK4	1.000 ALK4	1.000 ALK4	1.000	ALK4	1.000 M24C5	ALK4	ALK4
C560-21-4	2,3,3-trimethylpentane	ALK4	1.000 ALK4	1.000 ALK4	1.000 ALK4	1.000	ALK4	1.000 M233C5	ALK4	ALK4
C563-16-6	3,3-dimethylhexane	ALK4	1.000 ALK4	1.000 ALK4	1.000 ALK4	1.000	ALK4	1.000 OTH4	ALK4	ALK4
C590-73-8	2,2-dimethylhexane	ALK4	1.000 ALK4	1.000 ALK4	1.000 ALK4	1.000	ALK4	1.000 M22C5	ALK4	ALK4
C564-02-3	2,2,3-trimethylpentane	ALK4	1.000 ALK4	1.000 ALK4	1.000 ALK4	1.000	ALK4	1.000 OTH4	ALK4	ALK4
C1067-08-9	3-methyl-3-ethylpentane	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 OTH5	ALK4	ALK4
C50876-33-0	1,1,3,3-tetramethyl Cyclopentane	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 CYCOS	ALK5	ALK4
C1067-20-5	3,3-dimethylpentane	ALK4	1.000 ALK4	1.000 ALK4	1.000 ALK4	1.000	ALK4	1.000 OTH4	ALK4	ALK4
C16187-30-1	2,4,4-trimethylhexane	ALK4	1.000 ALK4	1.000 ALK4	1.000 ALK4	1.000	ALK4	1.000 OTH4	ALK4	ALK4
C3522-94-9	2,2,5-trimethylhexane	ALK4	1.000 ALK4	1.000 ALK4	1.000 ALK4	1.000	ALK4	1.000 M225C6	ALK4	ALK4
C1186-53-4	2,2,3,4-tetramethylpentane	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 BRC9	ALK5	ALK4
C3074-76-8	3-ethyl-3-methyl Hexane	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 BRC9	ALK5	ALK4
C508-32-7	tricyclene	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 OTH5	ALK4	ALK4
C107-16-4	hydroxyacetoneitrile	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 OTH5	OTH3	OTH3
C107-21-1	ethylene glycol	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 ETGLYCL	OTH4	OTH4
C75-18-3	dimethyl sulfide	ALK4	1.000 ALK4	1.000 ALK4	1.000 ALK4	1.000	ALK4	1.000 OTH4	OTH3	OTH3
C75-08-1	ethyl mercaptan	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 OTH5	OTH3	OTH3
C503-30-0	Trimethylene Oxide (1,3-epoxypro	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 OTH5	OTH4	OTH4
C646-06-0	1,3-dioxolane	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 OTH5	OTH4	OTH4
C109-85-4	2-methoxyethanol (methyl cellos	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 MEETOH	OTH4	OTH4
C57-55-6	propylene glycol	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 PRGLYCL	OTH4	OTH4
C56-81-6	glycerol	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 GLYCERL	OTH4	OTH4
C96-24-2	Glycerol alpha-monochlorohydrin	ALK4	1.000 ALK4	1.000 ALK4	1.000 ALK4	1.000	ALK4	1.000 OTH4	OTH3	OTH3
C107-00-6	1-butene (ethylacetylene)	OLE1	1.000 OLE1	1.000 OLE1	1.000 OLE1	1.000	OLE1	1.000 ETACTYL	ACYLS	ACYLS
C109-99-9	tetrahydrofuran	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 THF	OTH4	OTH4
C71-36-3	n-butyl alcohol	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 NCAOH	OTH3	OTH3
C78-92-2	sec-butyl alcohol	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 SCAOH	OTH3	OTH3
C78-83-1	isobutyl alcohol	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 IC4OH	OTH3	OTH3
C60-29-7	ethyl ether	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 ET0ET	OTH4	OTH4
C123-91-1	1,4-dioxane	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 OTH5	OTH4	ALK5
C110-63-4	1,4-butanediol	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 OTH5	OTH4	OTH4
C1320-67-8	3-methoxy-1-propanol	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 OTH5	OTH4	OTH4
C110-80-5	2-ethoxyethanol (cellosolve) (see	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 ETOEOTH	OTH4	OTH4
C107-98-2	propylene glycol methyl ether (1-n	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 MEC3OH	OTH4	OTH4
C513-85-9	2,3-Butanediol	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 OTH5	OTH4	OTH4
C1589-47-5	2-methoxy-1-propanol	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 OTH5	OTH4	OTH4
C584-03-2	1,2-butanediol	2-Butanediol	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 C4OH12	OTH4	OTH4
C107-88-0	1,3-butanediol	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 OTH5	OTH4	OTH4
C534-15-6	1,1-dimethoxy ethane	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 OTH5	OTH3	OTH3
C110-71-4	1,2-Dimethoxyethane	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 OTH5	OTH4	ALK5
C111-45-6	diethylene glycol (2,2'-oxybisetha	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 DETGLCL	OTH4	OTH4
C64-67-6	Diethyl Sulfate	ALK5	1.000 ALK5	1.000 ALK5	1.000 ALK4	1.000	ALK5	1.000 OTH5	OTH4	OTH4

Documentation Update history Parameters and Commands Master List Compounds Notes Atoms Mix Profile Assignments SAROAD assignments

Speciated emissions as model inputs



VOC monitoring and analysis

- ❑ Collect air in canisters
- ❑ 5 locations in Tokyo
- ❑ 2 days per season in 2019-2020
 - October 15 – 17 (Fall), December 9 – 11 (Winter), April 20 – 22 (Spring), and June 29 – July 1 (Summer)
- ❑ 3 times per day
 - 18 – 6, 6 – 12, and 12 – 18
- ❑ Identify 126 VOCs and 13 aldehydes



VOC air quality simulations

- Regional meteorological model
 - WRF-ARW version 4.2.1
- Regional chemical transport model
 - CMAQ version 5.3.2
- 3 nested target domains



d01 (45 x 45 km)



d02 (15 x 15 km)



d04 (5 x 5 km)



Target VOC species

	SAPRC07	Monitored VOC species
Alkane	ALK1	Ethane, Dichloromethane, 1,1-Dichloroethane, 1,2-Dichloroethane, 1,2-Dibromoethane, 1,1,2-Trichloroethane, Tetrachloroethylene
	ALK2	Propane, Ethylchloride, Methylacetate, Ethylacetate, 1,2-Dichloropropane
	ALK3	Isobutane, n-Butane, 2,2-Dimethylbutane, Methyl-t-butylether, c-1,2-Dichloroethylene, 2,2,4-Trimethylpentane, Trichloroethylene
	ALK4	Isopropanol, n-Propanol, Cyclopentane, 2-Methylbutane, n-pentane, Methylcyclopentane, 2,3-Dimethylbutane, 2-Methylpentane, 3-Methylpentane, n-Hexane, 2,4-Dimethylpentane, n-Heptane, 2,3,4-Trimethylpentane, Butylacetate
	ALK5	Acrylonitrile, Vinylchloride, Isobutanol, n-Butanol, 3-Chloro-1-propene, Cyclohexane, 1,1-Dichloroethene, Methylcyclohexane, 2-Methylhexane, 2,3-Dimethylpentane, 3-Methylhexane, Ethyl-t-butylether, c-1,3-Dichloropropene, t-1,3-Dichloropropene, 2-Methylheptane, 3-Methylheptane, n-Octane, n-Nonane, n-Decane, n-Undecane
Alkene	ETHENE	Ethylene
	PROPENE	Propylene
	BUTADIENE13	1,3-Butadiene
	OLE1	1-Butene, 1-Pentene, 3-Methyl-1-butene, 1-Hexene, 1-Heptene
	OLE2	c-2-Butene, t-2-Butene, Isobutene, c-1,3-Pentadiene, t-1,3-Pentadiene, c-2-Pentene, t-2-Pentene, 2-Methyl-1-butene, 2-Methyl-2-butene, 2-Methyl-1-pentene, c-3-Hexene, c-2-Hexene, t-2-Hexene, c-3-Methyl-2-pentene, t-3-Methyl-2-pentene, Styrene

Target VOC species

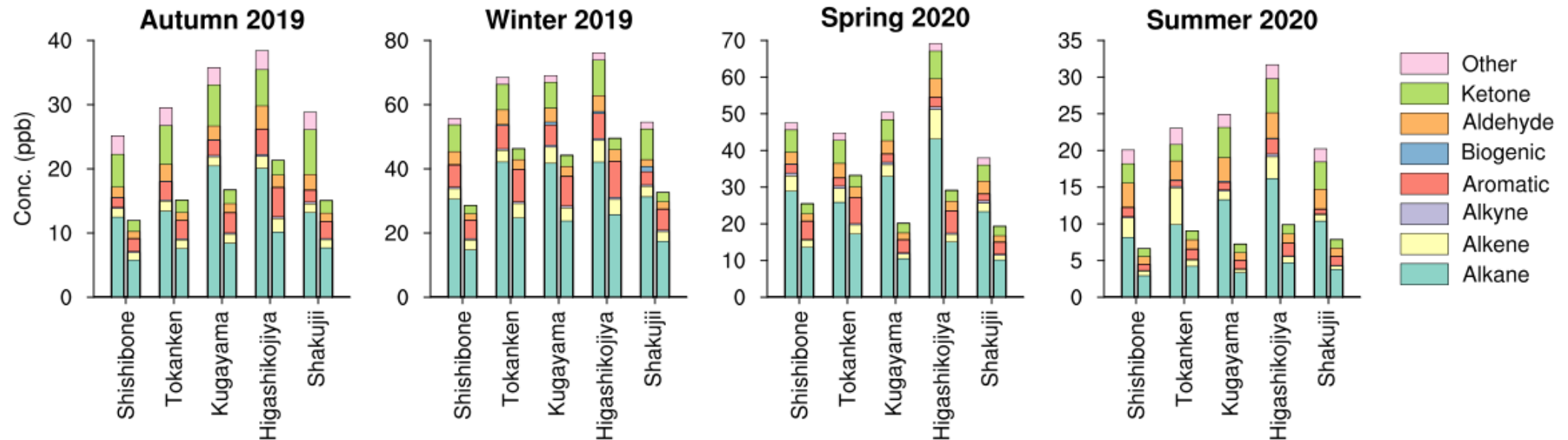
	SAPRC07	Monitored VOC species
Alkyne	ACETYLENE	Acetylene
Aromatic	BENZENE	Benzene
	TOLUENE	Toluene
	MXYL+PXYL	m,p-Xylene
	OXYL	o-xylene
	ARO1	Ethylbenzene, Chlorobenzene, Isopropylbenzene, Propylbenzene, Benzylchloride, m-Dichlorobenzene, p-Dichlorobenzene, o-Dichlorobenzene
	TMBENZ124	1,2,4-Trimethylbenzene
	ARO2	1,2,3-Trimethylbenzene, 1,3,5-Trimethylbenzene, m-Ethyltoluene, o-Ethyltoluene, p-Ethyltoluene, m-Diethylbenzene, p-Diethylbenzene, 2-Ethyl-p-xylene, 1,2,3,5-Tetramethylbenzene
Biogenic	ISOPRENE	Isoprene
	APIN	α -Pinene
	TERP	β -Pinene, Camphene, Limonene

Target VOC species

	SAPRC07	Monitored VOC species
Aldehyde	HCHO	Formaldehyde
	CCHO	Acetaldehyde
	ACROLEIN	Acrolein
	IPRD	Crotonaldehyde
	RCHO	Propionaldehyde, Butyraldehyde, Isovaleraldehyde, Valeraldehyde, Hexanaldehyde
	BALD	Benzaldehyde, o-Tolualdehyde, m,p-Tolualdehyde, 2,5-Dimethylbenzaldehyde
Ketone	ACETONE	Acetone
	MEK	Methylethylketone
	PRD2	Methylisobutylketone
Other	NROG	Chloromethane, Bromomethane, Chloroform, 1,1,1-trichloroethane, Carbontetrachloride, 1,1,2,2-Tetrachloroethane, 1,2,4-Trichlorobenzene, Hexachloro-1,3-butadiene, HCFC-22, HCFC-142, HCFC-141, CFC-12, CFC-11, HCFC-123, CFC-114, CFC-113, HCFC-225ca, HCFC-225cb

Comparison of monitored and simulated VOCs

- Total VOC concentrations at all locations for all periods were underestimated.
- Underestimations of alkanes and ketones are evident.



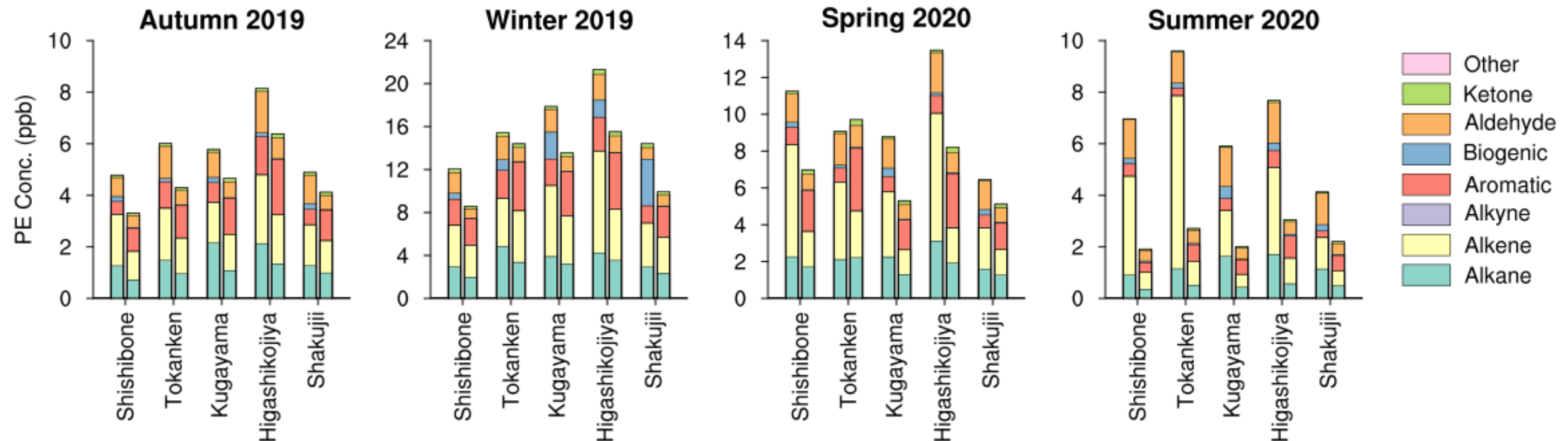
Monitored (left) and simulated (right) concentrations averaged for each period

Comparison of monitored and simulated VOCs

- Smaller deviations in propylene-equivalent (PE) concentrations considering reactivities in the atmosphere.

- $$PE \text{ concentration} = \text{Concentration} \times \frac{\text{Reaction rate with OH}}{\text{Reaction rate of propylene with OH}}$$

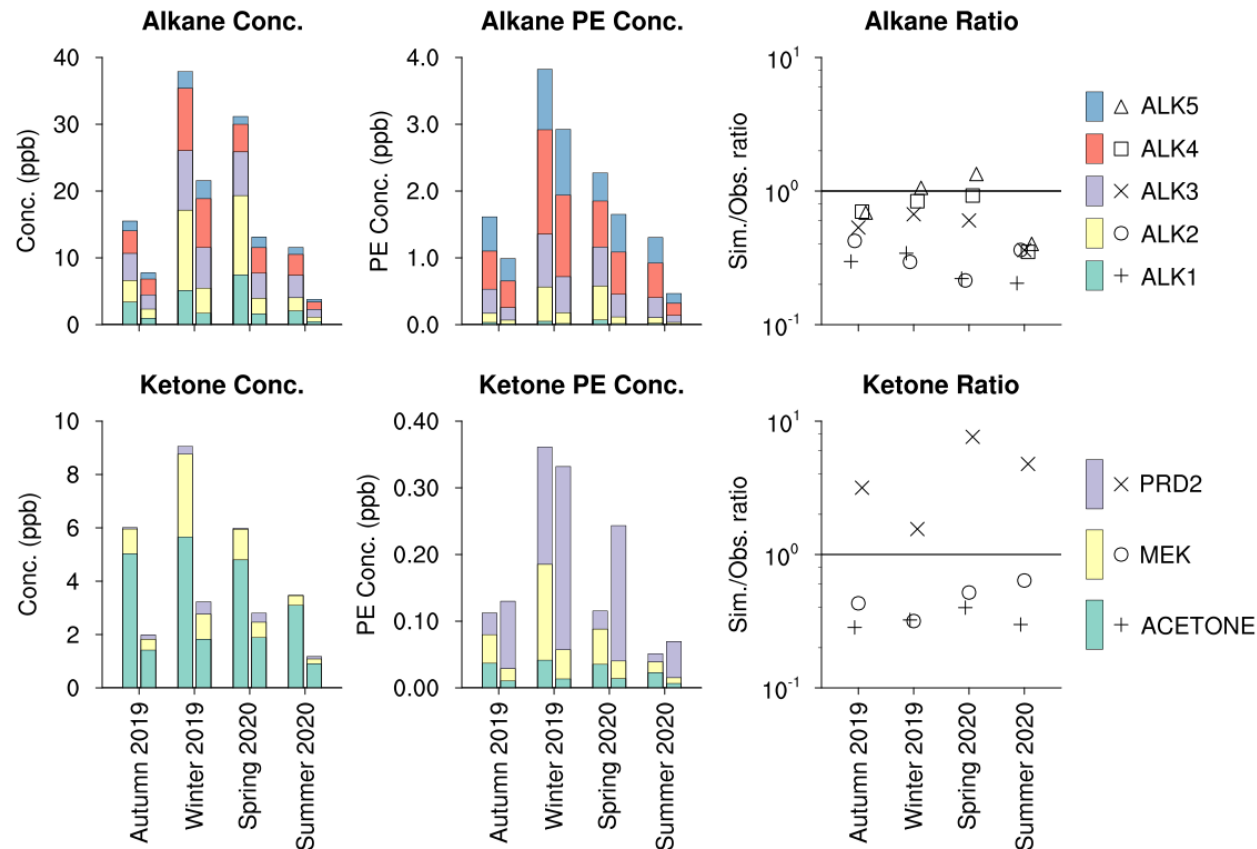
- Underestimation of alkenes and overestimation of aromatic are evident.



Monitored (left) and simulated (right) PE concentrations averaged for each period

Comparison of monitored and simulated VOCs

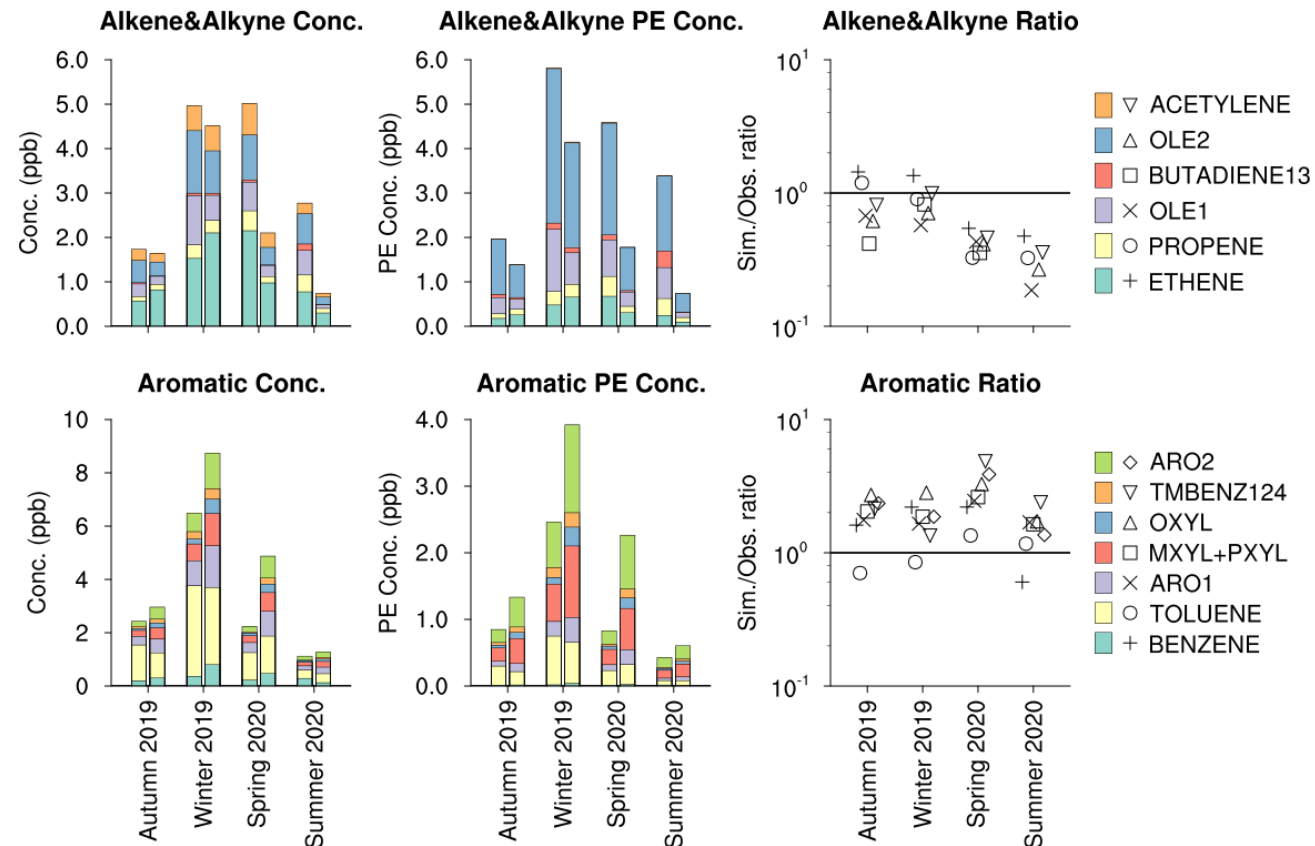
- Underestimations of smaller alkanes (mainly ethane and propane) and acetone are evident.



Monitored (left) and simulated (right) concentrations of alkanes and ketones averaged for each period

Comparison of monitored and simulated VOCs

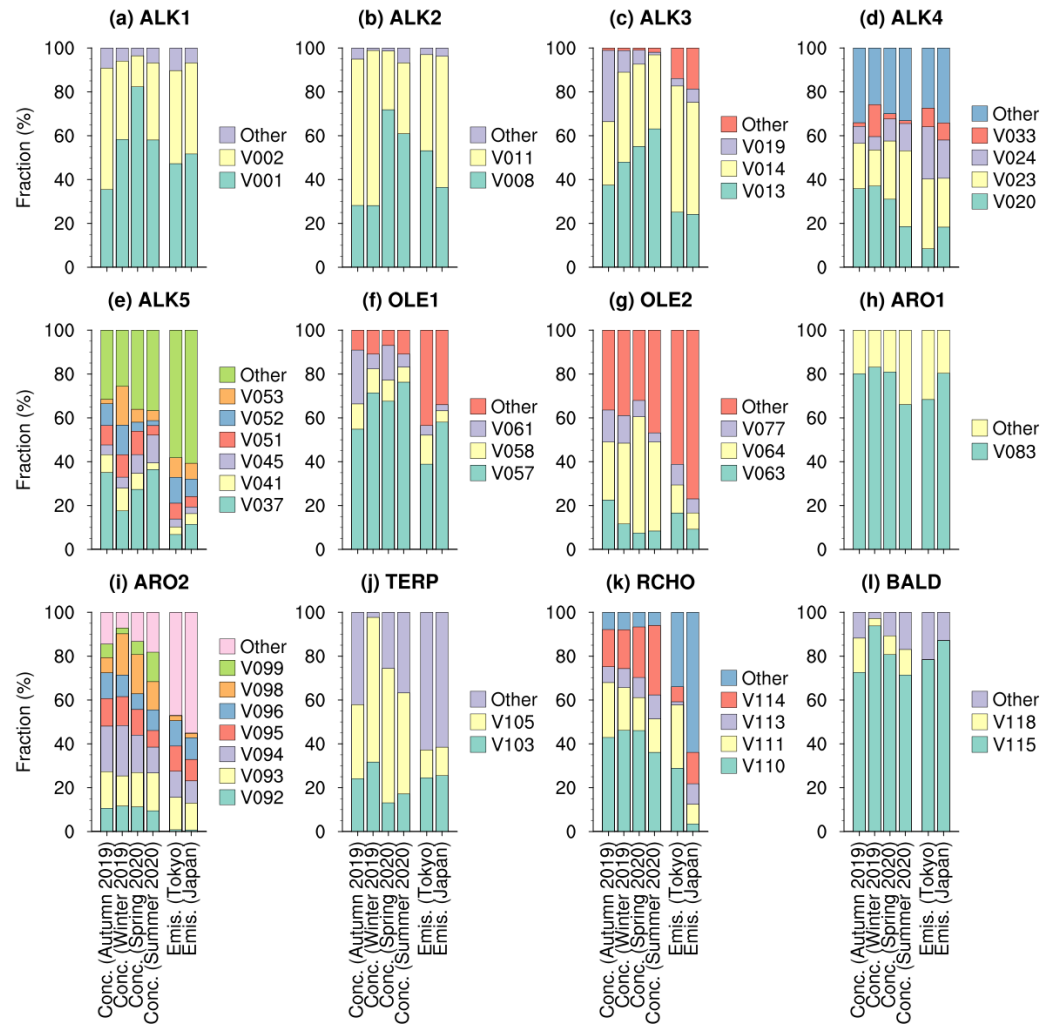
- Underestimations of OLE1 and OLE2, and overestimations of XYL and ARO2 are evident in PE concentrations.



Monitored (left) and simulated (right) concentrations of alkenes and aromatics averaged for each period

VOC compositions in monitoring and emissions

- VOC compositions in monitoring and emissions are generally consistent.



OLE1

V057: 1-Butene

OLE2

V064: Isobutene

ARO2

V093: 1,3,5-Trimethylbenzene

V094: m-Ethyltoluene

V095: o-Ethyltoluene

V096: p-Ethyltoluene

Fractions of individual VOC species in the monitored concentrations (left) and emissions (right)

Implications of VOC air quality simulations

- ❑ Validations of air quality simulations on VOC species are suggested whereas monitoring data of individual VOC species are limited.
- ❑ Uncertainties in emissions and models are clarified by air quality simulations.
- ❑ Information of individual VOC species is useful to identify problems in emissions and models.
- ❑ **Poor model performances on VOC species may introduce inappropriate ozone formation regimes.**

Summary

- ❑ Air quality modeling is essential to consider effective strategies for suppressing ambient concentrations of secondary pollutants.
- ❑ Representation of VOCs in chemical transport models is simplified in chemical mechanisms.
- ❑ VOC emissions need to be speciated to lumped species of chemical mechanisms based on speciation profiles.
- ❑ Observations of individual VOC species are useful to validate and improve air quality modeling of NMVOC.

**Thank you
for your attention**