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Supporting Information for

Impact of battery electric vehicle penetration and corresponding changes in upstream processes on summer O_3 concentrations in Japan

Satoko Kayaba[1,2] and Mizuo Kajino[2,3]

1 Graduate School of Science and Technology, University of Tsukuba, Tsukuba, Ibaraki 305-8572, Japan

2 Meteorological Research Institute (MRI), Japan Meteorological Agency (JMA), Tsukuba, Ibaraki 305-0052, Japan

3 Faculty of Life and Environmental Sciences, University of Tsukuba, Tsukuba, Ibaraki 305-8572, Japan

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Introduction

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- $(H_2O_2 + ROOH)/NO_z$ distributions (Fig. S4)
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- Details of the simulation setting in this study (Table. S1)
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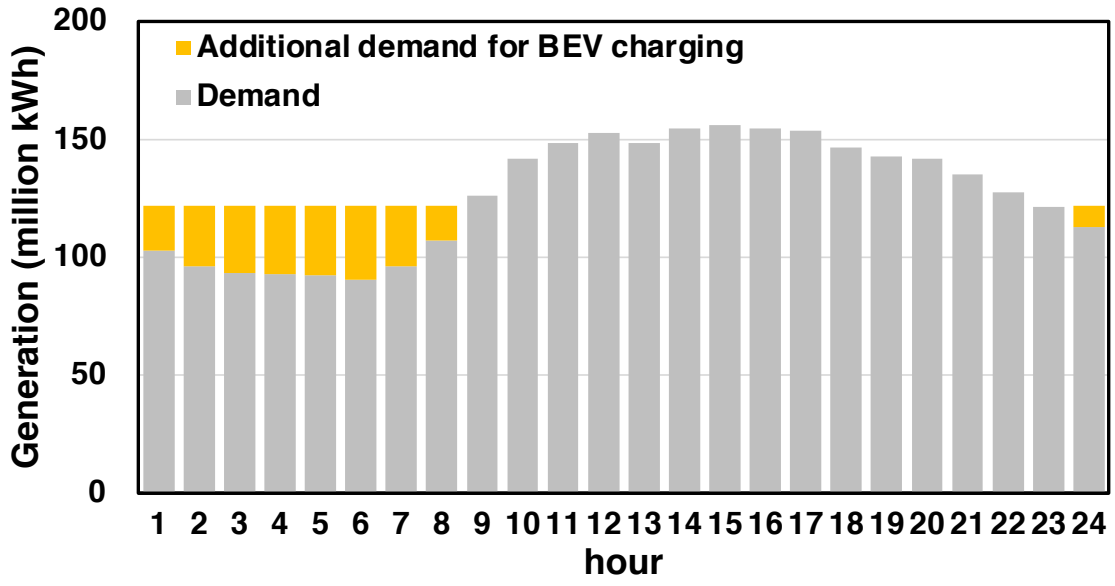

Figure S1. Additional electricity demand for BEV charging. The baseline demand is the demand pattern of July 27, 2012, which was used because the data were publicly available as electricity demand on the day of maximum electricity demand (according to the Power Companies of Japan: https://www.ene100.jp/zumen/1-2-10, last accessed: July 1, 2022). The additional demand was derived by the method in Section 2.2.2 of the main text.

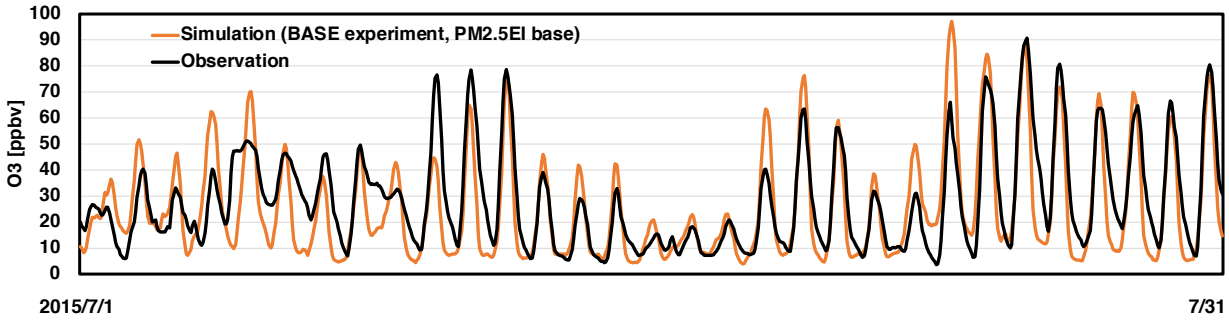

Figure S2. Time series of O_3 concentrations in Kanto in July 2015. Comparison of observation data (black line) and model simulation results (orange line).

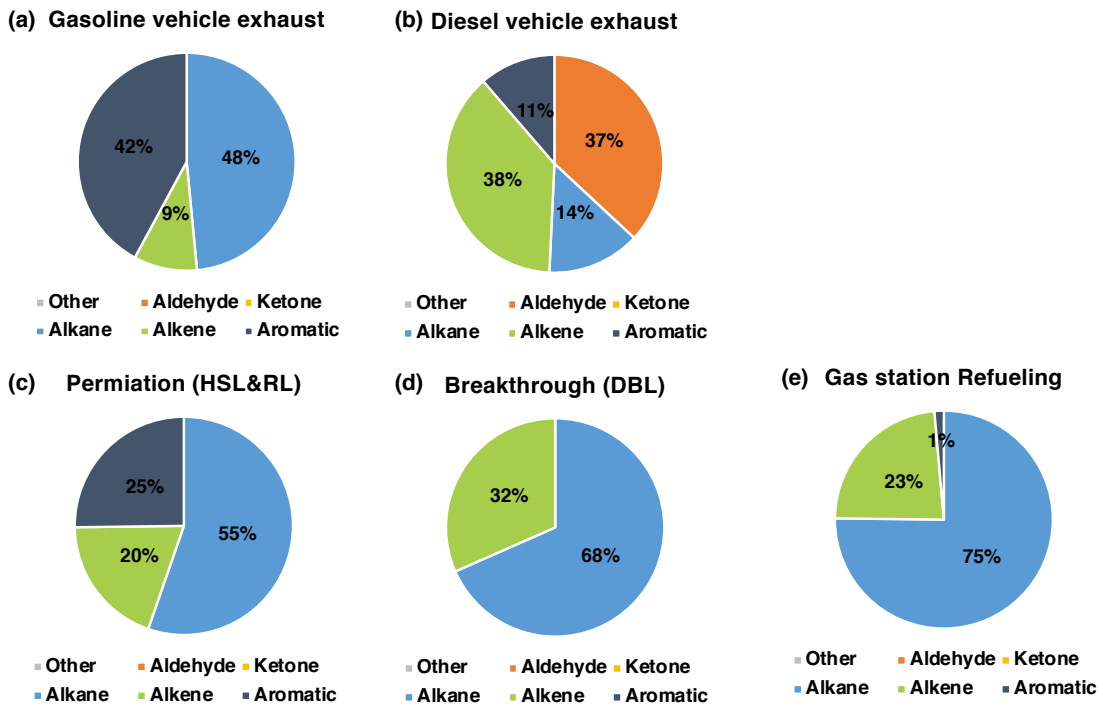

Figure S3. VOC profiles for each source. The components of exhaust gas in gasoline and diesel vehicles are the results of the tunnel survey by *Uchida et al.* (2013). The component of DBL is the result of the DBL test by *Yamada et al.* (2015a) after day 2 (caused by breakthrough). The component of HSL & RL is the result of the DBL test by *Yamada et al.* (2015a) on day 1 (caused by permeation). We determined that these data could be used because HSL & RL is mainly caused by the transmission. The component of refueling is the results of the test by *Yamada et al.* (2015b).

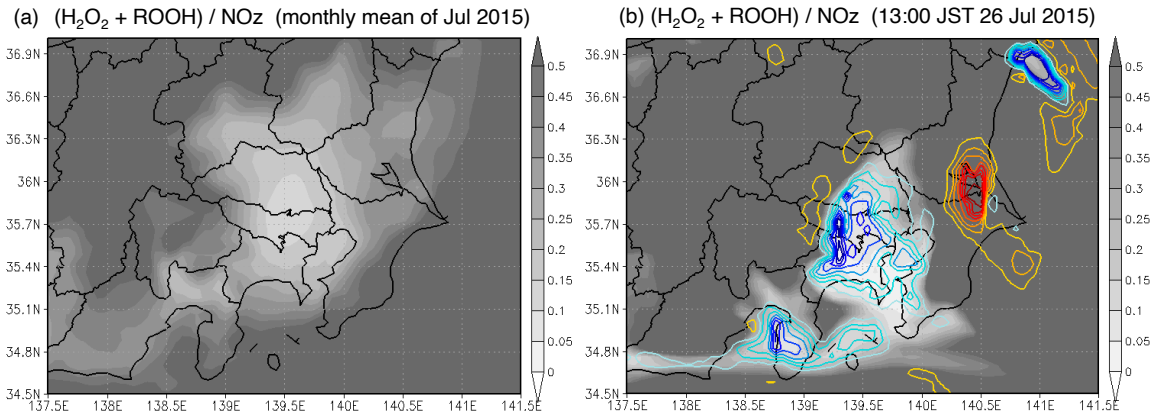

Figure S4. Same as Figure 8 but for (H_2O_2 + ROOH)/NOz.

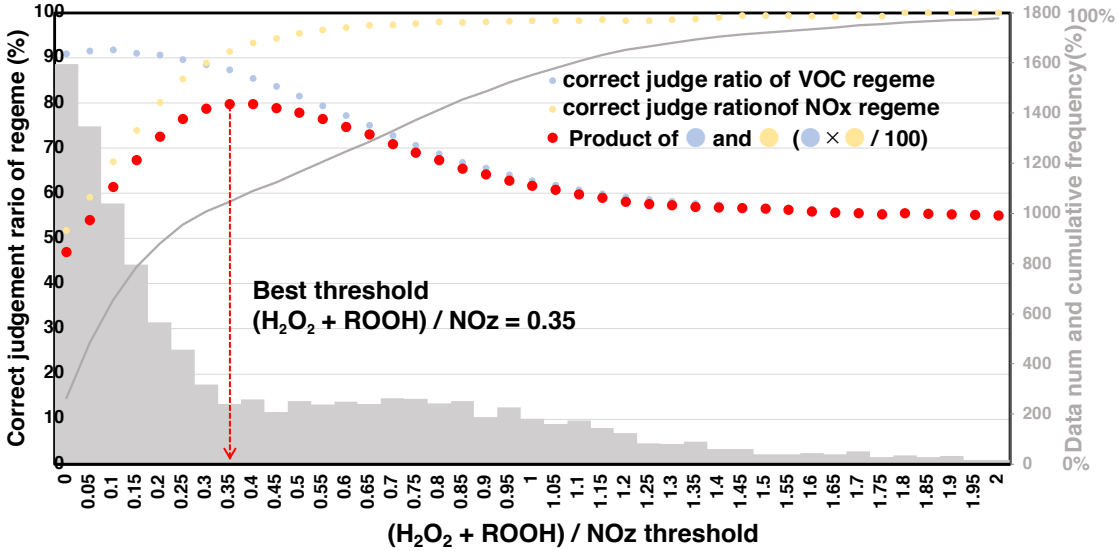

Figure S5. This is the same as Figure A1 but for (H_2O_2 + ROOH)/NOz.

Table S1. Simulation setting in this study

Model	Offline NHM-Chem[a] (*Kajino et al.,* 2019; *Kajino et al.,* 2021)	
Region	Domain 1: East Asia (dx = 30 km) Domain 2: Japan from Kyusyu to Tohoku (dx = 6 km)	
Period	From July 1 to 31, 2015	
Boundary conditions of NHM	Reanalysis data Domain 1: JRA-55, 6 hourly (*Kobayashi et al.,* 2015) Domain 2: JMA's Meso-Regional Objective Analysis (MA), 3 hourly (https://www.jma.go.jp/jma/jma-eng/jma-center/nwp/nwp-top.htm, last accessed: 30 July 2022).	
Boundary conditions of CTM[b]	Domain 1: monthly climatological data simulated by a global model Gases : MRI-CCM2 (*Deushi and Shibata,* 2011) Aerosols: MASINGAR-mk2 (*Tanaka et al.,* 2003; *Tanaka and Ogi,* 2017; *Yumimoto et al.,* 2017;) Domain 2: Domain 1	
Time intervals	1 h (output of NHM and input/output of CTM)	
Emission	Anthropogenic	East Asia: REASv3.2.1 (2015 base) (*Kurokawa and Ohara,* 2020) *REASv3.2.1 was updated from v3.2 in Dec 2021. Japan: PM2.5EI (2012 base) (*Morikawa,* 2017) + EAGrid for navigation (2010 base) (*Fukui et al.,* 2014; *Kannari et al.,* 2007)
	Biomass burning	GFED v4 (*Giglio et al.,* 2013)
	Biogenic VOC	MEGAN v2 (*Guenther et al.,* 2006)
	Volcano SO_2	Observation data of JMA
	Mineral dust	Inline calculation based on the method of *Han et al.* (2004)
	Sea salt	Inline calculation based on the method of *Clark et al.* (2006)

a. NHM-Chem is coupled with the meteorological model NHM offline or online. In the case of offline coupling, drive NHM first and then the chemical transport model using the results of the meteorological simulation.
b. Chemical transport model (CTM) part of NHM-Chem

Table S2. List of MIR for the SUPRC-99 VOC group (derived regarding Carter, 2000)

Name	name description in NHM-Chem	weighted MIR ($g\text{-}O_3$/ g-NMVOC)	weighted MIR ($mol\text{-}O_3$/ mol-NMVOC)	species	Weight %	MIR ($g\text{-}O_3$/g-NMVOC)	MWT (g-NMVOC/mol-NMVOC)
hcho	formaldehyde	9.27	5.80	formaldehyde	100.0	9.27	30.03
meoh	methanol	0.77	0.51	methanol	100.0	0.77	32.04
mek	ketones and other non-aldehyde oxygenated products (slower with OH)	1.70	3.05	Cyclobutanone	12.5	0.77	70.09
				Methyl Ethyl Ketone	12.5	1.59	72.11
				Cyclopentanone	12.5	1.51	84.12
				3-Pentanone	12.5	1.55	86.13
				2-Pentanone	12.5	3.34	86.13
				Methyl t-Butyl Ketone	12.5	0.86	100.16
				Hydroxy Acetone	12.5	3.22	74.08
				Diacetone Alcohol	12.5	0.76	116.16
prod2	ketones and other non-aldehyde oxygenated products (faster with OH than 5e-12 cm3/molec2/sec)	2.45	6.02	Cyclohexanone	9.1	1.76	98.15
				4-Methyl-2-Pentanone	9.1	4.62	100.16
				Methyl n-Butyl Ketone	9.1	3.82	100.16
				Di-Isopropyl Ketone	9.1	1.80	114.19
				2-Methyl-3-Hexanone	9.1	1.98	114.19
				2-Heptanone	9.1	3.05	114.19
				2-Octanone	9.1	1.81	128.22
				2-Nonanone	9.1	1.42	142.24
				Di-isobutyl ketone (2,6-dimethyl-4-heptanone)	9.1	3.22	142.24
				2-Decanone	9.1	1.14	156.27
				Methoxy Acetone	9.1	2.33	88.11
cco_oh	acetic acid	0.83	1.05	Acetic Acid	100.0	0.83	60.5
ccho	acetaldehyde	7.25	6.65	acetaldehyde	100.0	7.25	44.05
acet	acetone	0.45	0.54	Acetone	100.0	0.45	58.08
phen	phenol	1.89	3.71	Phenol	100.0	1.89	94.11
hcooh	formic acid	0.09	0.05	Formic Acid	100.0	0.09	30.03
rcho	lumped c3 + aldehydes	5.65	11.03	Propionaldehyde	6.7	8.43	58.08
				2-Methylpropanal	6.7	6.30	72.11
				Butanal	6.7	7.15	72.11
				Pentanal	6.7	6.10	86.13
				2,2-Dimethylpropanal	6.7	5.78	86.13
				3-Methylbutanal	6.7	5.91	86.13
				Glutaraldehyde	6.7	5.18	100.12
				Hexanal	6.7	5.17	100.16
				Heptanal	6.7	4.40	114.19
				Octanal	6.7	3.79	128.22
				C4 aldehydes	6.7	7.15	72.11
				C5 aldehydes	6.7	6.10	86.14
				C6 aldehydes	6.7	5.17	100.16
				C7 aldehydes	6.7	4.40	114.19
				C8 aldehydes	6.7	3.79	128.22
gly	glyoxal	14.81	17.91	Glyoxal	100.0	14.81	58.04
mgly	methyl glyoxal	16.99	25.51	Methyl Glyoxal	100.0	16.99	72.07
bacl	biacetyl	21.75	39.01	Biacetyl	100.0	21.75	86.09
cres	cresols	2.41	5.43	m-cresol	33.3	2.41	108.14
				p-cresol	33.3	2.41	108.14
				o-cresol	33.3	2.41	108.14
bald	aromatic aldehydes (e.g. benzaldehyde)	-0.51	-1.13	Benzaldehyde	100.0	-0.51	106.13
methacro	methacrolein	6.67	9.74	Methacrolein	100.0	6.67	70.09
mvk	methyl vinyl ketone	10.05	15.10	Methylvinyl ketone	100.0	10.05	72.11
isoprod	lumped isoprene product species	8.53	13.87	Crotonaldehyde	50.0	10.34	70.09
				Hydroxy Methacrolein	50.0	6.71	86.09
ethene	ethene	9.53	5.57	ethene	100.0	9.53	28.05
isoprene	isoprene	11.48	16.29	isoprene	100.0	11.48	68.12
trp1	terpens	4.05	11.61	a-Pinene	38.0	4.51	136.24

				b-Pinene	27.0	3.58	136.24
				3-Carene	17.0	3.47	136.24
				Sabinene	10.0	3.96	136.24
				d-Limonene	9.0	4.25	136.24
ALK1	alkanes and other non-aromatic comp., react only with OH, kOH < 5.e2 /ppm/min) :: almost ethane	0.35	0.22	ethane	100.0	0.35	30.07
ALK2	alkanes and other non-aromatic comp., react only with OH, kOH < 2.5e3	0.91	0.70	propane	59.0	0.64	44.1
				acetylene	41.0	1.31	26.04
ALK3	alkanes and other non-aromatic comp., react only with OH, kOH < 5.e3	1.48	1.81	n-butane	68.0	1.48	58.12
				isobutane	30.0	1.48	58.12
				2,2-dimethylbutane	2.0	1.45	86.18
ALK4	alkanes and other non-aromatic comp., react only with OH, kOH < 1. e4	1.95	3.18	isopentane	45.0	1.87	72.15
				n-pentane	18.0	1.77	72.15
				2-methylpentane	11.0	2.02	86.18
				3-methyl pentane	8.0	2.33	86.18
				2,4-dimethylpentane	5.0	1.90	100.21
				methylcyclopentane	5.0	2.46	84.16
				n-hexane	4.0	1.71	86.18
				2,3-dimethyl butane	3.0	1.28	86.18
				cyclopentane	2.0	2.65	70.14
ALK5	alkanes and other non-aromatic comp., react only with OH, kOH > 1. e4	1.53	3.65	2,4-Dimethyl Hexane	11.0	2.13	114.23
				n-Decane	10.0	0.97	142.29
				3-Methyl Hexane	10.0	1.66	100.21
				n-Heptane	7.0	1.48	100.21
				2,3-Dimethyl Pentane	6.0	1.75	100.21
				2-Methyl Heptane	6.0	2.02	114.23
				4-Methyl Heptane	6.0	1.67	114.23
				2,4-Dimethyl Heptane	5.0	1.75	128.26
				Methylcyclohexane	4.0	2.09	98.19
				2,6-Dimethyl Octane	4.0	1.44	142.29
				n-Nonane	4.0	1.10	128.26
				n-Octane	4.0	1.28	114.23
				Cyclohexane	4.0	2.02	84.16
				2-Methyl Hexane	3.0	1.74	100.21
				4-Methyl Octane	2.0	1.31	128.26
				2-Methyl Octane	2.0	1.15	128.26
				4-Methyl Nonane	2.0	1.18	142.29
				2-Methyl Nonane	2.0	1.02	142.29
				n-Dodecane	2.0	0.81	170.34
				Ethylcyclohexane	1.0	1.95	112.22
				n-Undecane	1.0	0.88	156.31
				3,6-Dimethyl Decane	1.0	1.03	170.34
ARO1	aromatics with kOH < 2.e4 /ppm/min	3.64	7.00	Toluene	70.0	4.24	92.14
				n-Propyl Benzene	10.0	2.40	78.11
				Ethyl Benzene	10.0	3.03	106.17
				Benzene [a]	7.0	0.91	78.11
				s-Butyl Benzene	2.0	2.15	134.22
				Isopropyl Benzene (cumene)	1.0	2.53	120.2
ARO2	aromatics with kOH > 2.e4 /ppm/min	9.06	21.21	m-Xylene	22.0	11.40	106.17
				p-Xylene	22.0	4.56	106.17
				o-Xylene	20.0	7.87	106.17
				1,3,5-Trimethyl Benzene	14.0	11.76	120.2
				1,2,3-Trimethyl Benzene	14.0	11.74	120.2
				1,2,4-Trimethyl Benzene	9.0	7.57	120.2
ORE1	alkenes with kOH < 7.e4 /ppm/min	8.19	12.42	Propene	29.0	12.19	42.08
				1-Hexene	24.0	6.09	84.16

	(other than ethene)			1-Butene	12.0	10.91	56.11
				1-Pentene	11.0	8.00	70.14
				1-Heptene	11.0	4.49	98.19
				1-Nonene	5.0	2.82	126.24
				3-Methyl-1-Butene	3.0	7.72	70.14
				1-Octene	2.0	3.42	112.22
				1-Undecene	2.0	2.09	154.3
				1-Decene	1.0	2.39	140.27
ORE2	alkenes with kOH > 7.e4 /ppm/min	9.49	14.74	trans-2-Pentene	13.0	10.86	70.14
				cis-2-Pentene	13.0	10.86	70.14
				trans-2-Butene	10.0	14.51	56.11
				Isobutene	10.0	6.59	56.11
				cis-2-Butene	8.0	13.81	56.11
				2-Methyl-1-Butene	8.0	6.78	70.14
				Styrene	7.0	2.17	104.15
				1,3-Butadiene	5.0	12.88	54.09
				2-Methyl-2-Butene	4.0	14.97	70.14
				Trans-2-Hexene	4.0	8.69	84.16
				Cis-2-Hexene	4.0	8.69	84.16
				Trans-3-Heptene	4.0	7.26	84.16
				Trans-4-Nonene	2.0	4.96	128.26
				Trans-4-Octene	2.0	6.02	112.22
				Trans-2-Heptene	2.0	7.10	98.19
				Trans-5-Undecene	2.0	3.73	154.3
				Cyclohexene	1.0	5.47	82.15
				Trans-4-Decene	1.0	4.27	140.27