

# Sensitivity Analysis of Individual VOC Species to Reduction of Atmospheric Ozone

Kouhei Yamamoto<sup>1)</sup>, Kazuo Nakajima<sup>1)</sup>, and Hikari Shimadera<sup>2)</sup>

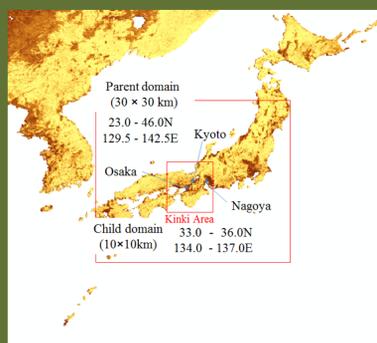
1) Graduate School of Energy Science, Kyoto Univ., Japan

2) Center for Environmental Innovation Design for Sustainability, Osaka Univ., Japan

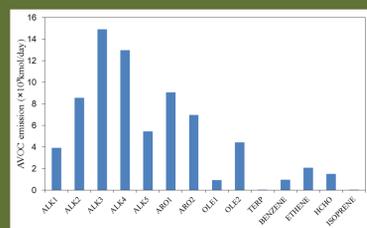
## Outline

- The sensitivities of anthropogenic VOCs to the reduction of atmospheric ozone in Kinki area, Japan were investigated by using CMAQv5.0.1 with WRFv3.4.1.
- Emission inventories of precursors were introduced from JATOP (Japan AuTo-Oil Program), and MEGANv2.04 for biogenic sources.
- SAPRC-99 model was adopted in CMAQ for gas phase chemistry.
- The sensitivity analysis of VOCs to ozone reduction in the child domain was conducted by estimating the change rates (CRs) of ozone concentrations in case of using 20 % reduced emission of each VOC species.
- Seven species of VOCs such as ALK3, ALK4, ARO1, ARO2, OLE2, ETHENE, HCHO were selected for sensitivity analysis, and the CR of each grid was sorted by values of each VOC concentration divided by NOx concentration.
- As remarkable decreases were shown in case of the reduction of former five species, the sum of five VOCs divided by NOx was proposed as a photochemical index for ozone reduction.
- The CRs under various ranges of ozone peak concentrations were estimated as a function of this developed index, and in the case that the index was below 0.2, the reduction rates were more prominent.

## Model Domain

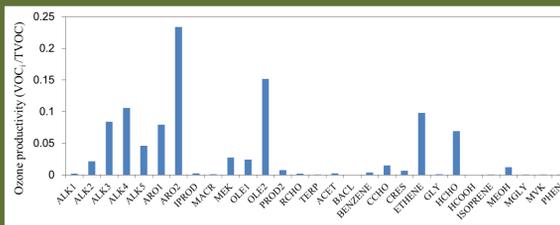


## VOCs emission in Kinki area



## Pre-estimation of ozone productivity P of VOCs

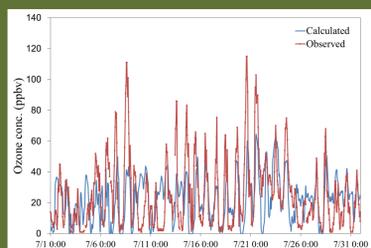
$$P = (MIR_i * VOC_i) / \sum (MIR_i * VOC_i)$$



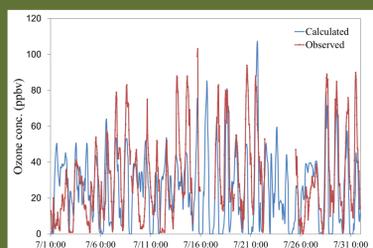
## VOCs in SAPRC99

SAPRC99	Description	N
ALK1	Alkanes that react with OH, $k_{OH} < 5 \times 10^2$ / (ppm·min)	10
ALK2	Same as ALK1, but $k_{OH} = 5 \times 10^2 \sim 2.5 \times 10^3$ (ppm·min)	16
ALK3	Same as ALK1, but $k_{OH} = 2.5 \times 10^3 \sim 5 \times 10^3$ (ppm·min)	23
ALK4	Same as ALK1, but $k_{OH} = 5 \times 10^3 \sim 1 \times 10^4$ (ppm·min)	32
ALK5	Same as ALK1, but $k_{OH} > 1 \times 10^4$ (ppm·min)	286
ARO1	Aromatics with $k_{OH} < 2 \times 10^1$ (ppm·min)	16
ARO2	Aromatics with $k_{OH} > 2 \times 10^1$ (ppm·min)	43
IPROD	Lumped isoprene product species	2
MACR	Methacrolein	2
MEK	Ketones and other oxygenated products with $k_{OH} > 5 \times 10^{-12}$ (ppm·min)	9
OLE1	Alkenes with $k_{OH} < 7 \times 10^4$ (ppm·min)	38
OLE2	Alkenes with $k_{OH} > 7 \times 10^4$ (ppm·min)	90
PROD2	same as MEK, but $k_{OH} > 5 \times 10^{-12}$ (ppm·min)	23
RCHO	Lumped C3+ aldehyde	14
TERP	Terpenes	6
ACET	Acetone	1
BACL	Biacetyl	1
BENZENE	Benzene	1
CCHO	Acetaldehyde	1
CRES	Cresols	1
ETHENE	Ethane	1
GLY	Glyoxal	1
HCHO	Formaldehyde	1
HCOOH	Formic acid	1
ISOPRENE	Isoprene	1
MEOH	Methanol	1
MGLY	Methyl glyoxal	1
MVK	Methyl vinyl ketone	1
PHEN	Phenol	1

## CMAQ performance



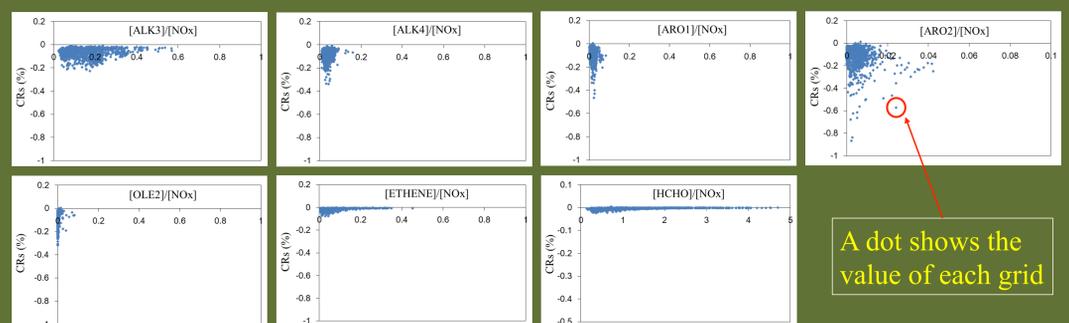
Osaka



Nagoya

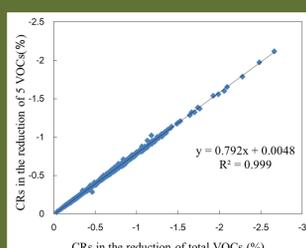
## Sensitivity analysis of individual VOC to CR

$$CR (\%) = 100 \times (C_{reduced} - C_{original}) / C_{original}$$

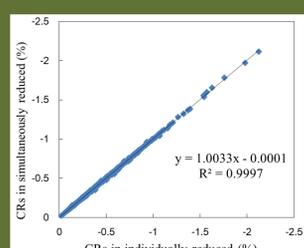


A dot shows the value of each grid

## Linearity of individual VOC to ozone reduction



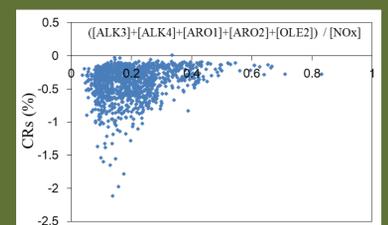
Comparison of CR in selected 5 VOCs with CR in total VOCs



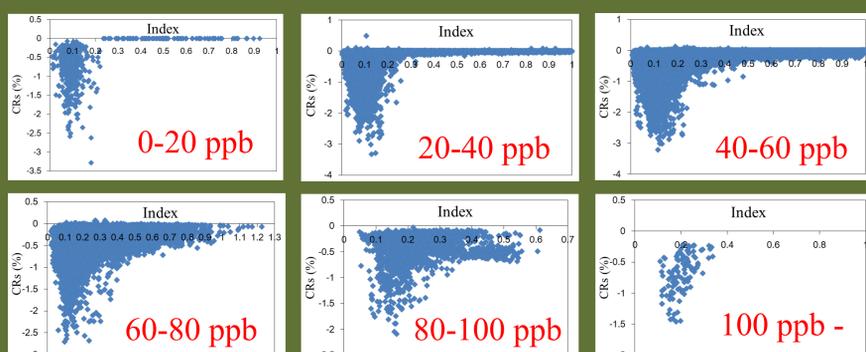
Comparison of summed CR in individually reduced with CR in simultaneously reduced

## CR and the developed Index

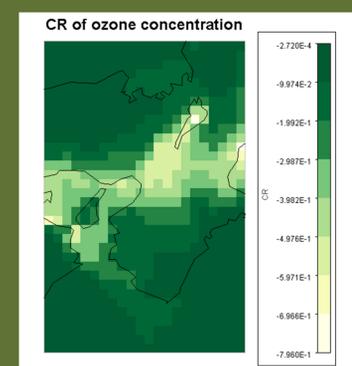
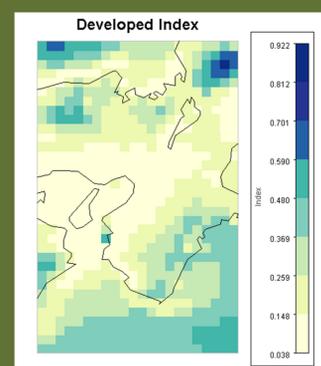
$$\text{Developed Index} = \frac{\{[ALK3] + [ALK4] + [ARO1] + [ARO2] + [OLE2]\}}{[NOx]}$$



## Availability of the index under various ranges of peak concentration



## Distribution of the index and relationship with CR



## Acknowledgement

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CR