Evaluation of differences in ozone concentration between chemical mechanisms of CMAQ in Japan

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Introduction

- The difference of ozone concentration between chemical mechanisms in the CMAQ model were evaluated for understanding errors caused by the selection of chemical mechanisms and factors of them.
- The process analysis was used for focusing the chemical process of ozone and the chemical reaction related with the difference of the chemical mechanisms.

Methods

Model settings

Model	Meteorological model	Chemical mechanism	Aerosol scheme
CMAQ v5.0.2	WRF v3.7.1	CB05tucl	AERO6
		RACM2	AERO6
		SAPRC07tc	AERO6
		SAPRC99	AERO5

Domain

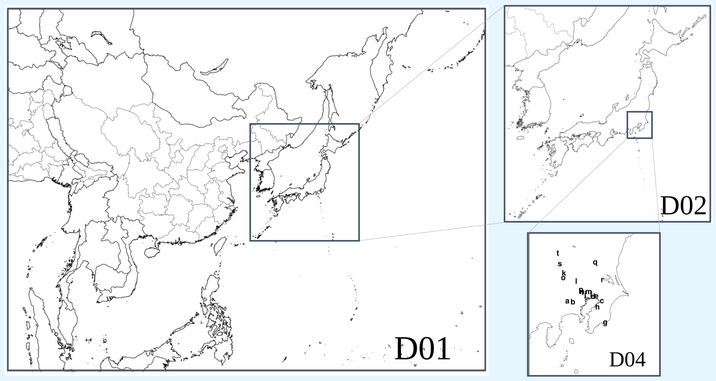

Fig. 1 Domains of the model calculation.
Domain 1 (D01) is the Asian region of 45 km grids. Domain 2 (D02) is the Japan region of 15 km grids. Domain 4 (D04) is the Kanto region of 5 km grids. Alphabet in D04 shows the location of observation site.

Target period: 2013/7/22 ～ 2013/8/10

Process analysis

The process analysis tool in CMAQ was used for calculating the Integrated Process Rate (IPR) of chemical processes of ozone and the Integrated Reaction Rate (IRR) of chemical reactions related to the ozone concentration. IPR and IRR were compared between the chemical mechanisms for detecting factors of the ozone concentration differences.

Results

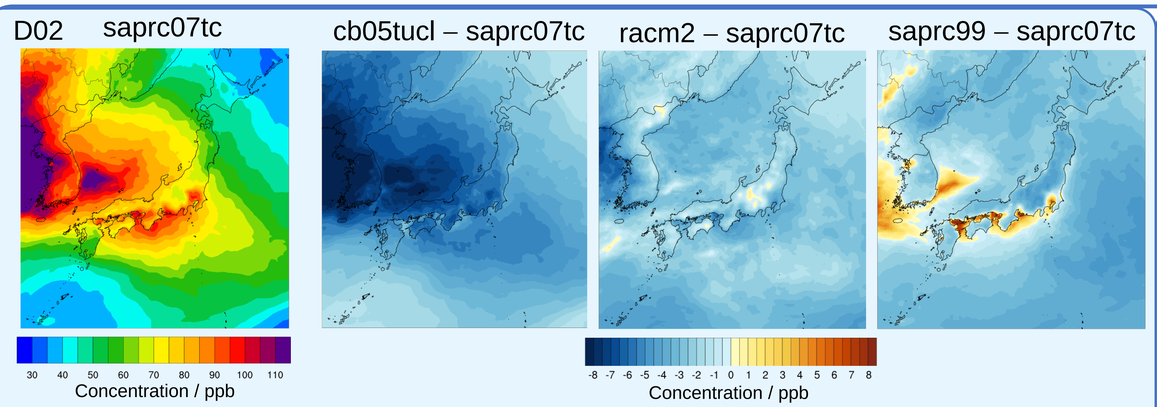

Fig. 2 Distribution of averaged day max ozone concentration in D02 for saprc07tc and the difference of averaged day max ozone concentration between saprc07tc and the other chemical mechanisms.

Ozone concentration of cb05tucl was lower than that of saprc07tc (Fig. 2). The difference was large in the high ozone concentration. The concentration of racm2 was higher in the terrestrial area and lower in the sea and urban area than that of saprc07tc. The concentration of saprc99 was higher in the urban area and lower in the sea and terrestrial area.

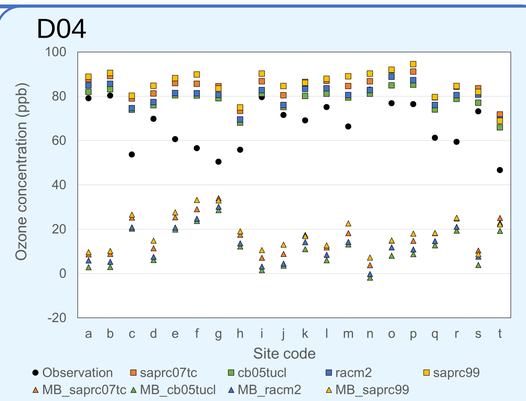

Fig. 3 Average of day max ozone concentration and the mean bias (MB) for the chemical mechanisms at the observation sites in D04.
Squares show the average of the daily max concentration for the target period. Triangles mean MB which is the mean of the difference of the daily max concentrations between observations and models.

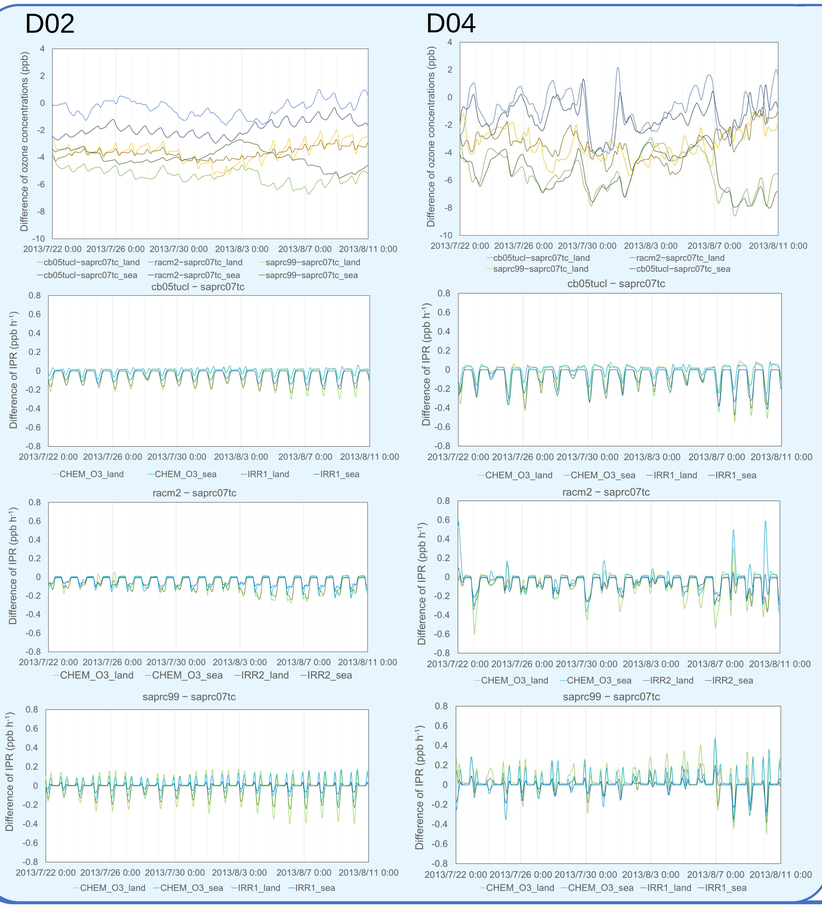

Fig. 4 Difference of hourly ozone concentration, IPR of the ozone chemical process and IRR of the chemical reaction related to ozone chemical process in D02 and D04 between saprc07tc and the other chemical mechanisms.
The concentration, IPR and IRR were averaged in D02 and D04 from surface to 10th vertical layers (approximately 3000 m above ground) divided in the land and sea areas. IPR and IRR were shown in hourly changes in the ozone concentration. CHEM_O3 means IPR of the ozone chemical process. The selected chemical reaction was the reaction most highly correlated with IPR of the ozone chemical process in the reactions related to ozone. IRR1 means IRR of the reaction, NO + HO_2 → NO_2 + OH. IRR2 means IRR for the reaction, RO_2 + NO → NO_2. These IRRs were multiplied by −1 in consideration of the reaction, O_3 + NO → NO_2 + O_2.

The difference of day max ozone concentration averaged in the target period between the models and observation ranged from −2 to 34 ppb at the observation sites in D04 (Fig. 3). The difference between the models were from 0.1 to 10 ppb.

The IRR of the reaction between NO and RO_2 and the following reaction between NO and HO_2 showed a good correlation with ozone chemical processes. Ozone chemical processes differed between the land and sea (Fig.4).

Conclusions

- In the chemical mechanisms, the ozone concentration in the surface of D04 showed the following relation: cb05tucl < racm2 < saprc07tc < saprc99
- The difference of ozone chemical processes was related with the difference of reaction rates for the reactions between NO and RO_2.

Acknowledgement
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