

The Influence of Atmospheric Conditions on the Production of Ozone during VOC Oxidation

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Background

- ▶ Surface temperatures predicted to increase due to climate change.
- ▶ What are the effects of increased temperatures on air quality?
 - ▶ Increased emissions from vegetation (BVOCs).
 - ▶ Increased reaction rates atmospheric chemistry.
 - ▶ ...
- ▶ Ozone is produced from the photochemistry of emitted NO_x and VOC, with VOC being the “fuel” and NO_x the “catalyst” for ozone production.
- ▶ Due to the photochemical nature of ozone production, meteorological factors such as temperature are drivers for ozone production.
- ▶ What are the effects of increased temperatures on tropospheric ozone concentrations?
 - ▶ Increased VOC emissions, especially

Motivation

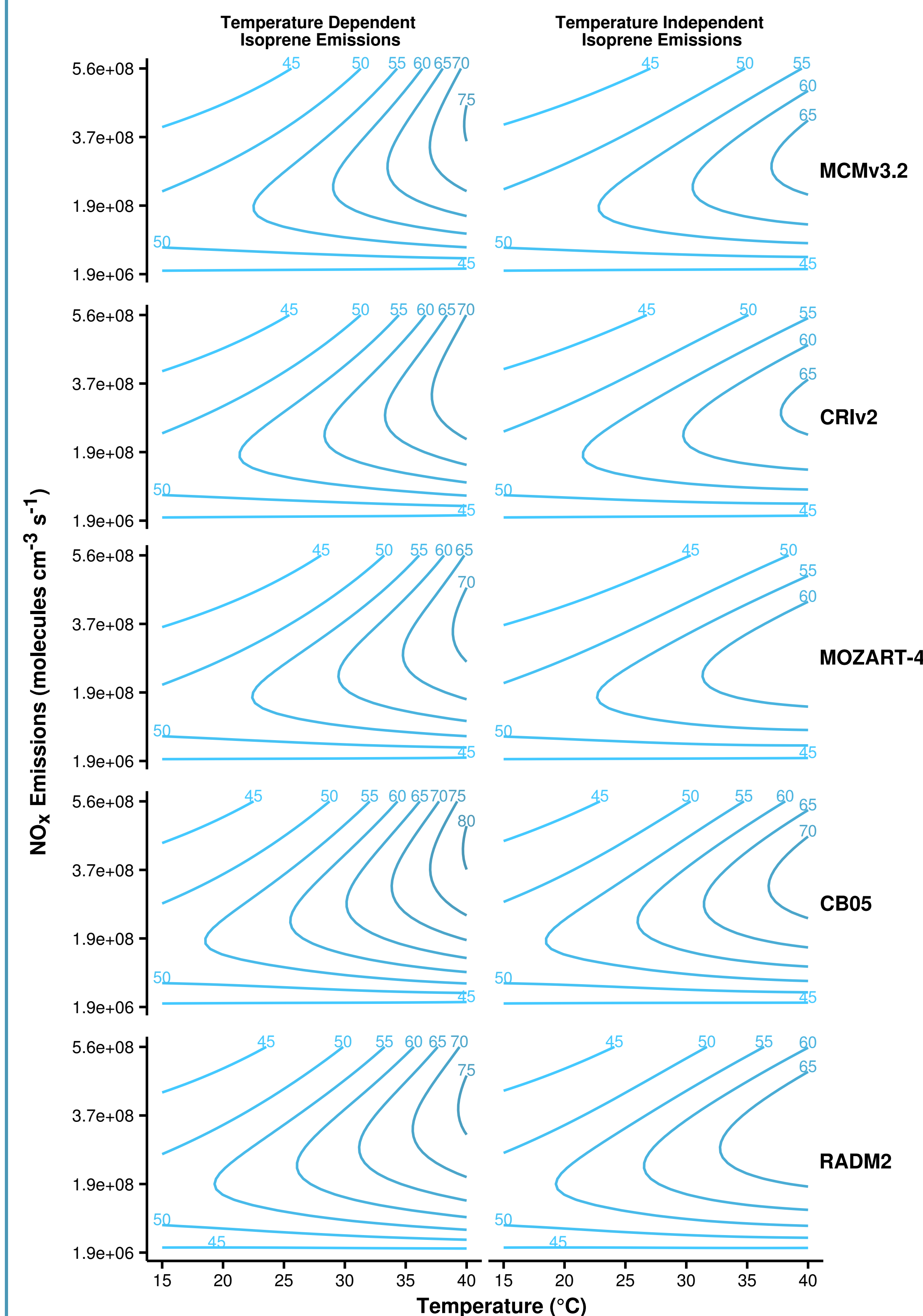
- ▶ Ozone levels over central europe are known to be driver by temperature. i.e. increases in temperature correlate with increases in ozone.
- ▶ Also confirmed in many studies over western and eastern US.
- ▶ This correlation is shown in many observational studies but modelling

Approach

- ▶ Idealised box model simulating central europe (Benelux).
- ▶ Systematic variations in NO_x over temperature range (15 – 40 °C).
- ▶ Simulations repeated using temperature dependent and independent source of isoprene emissions

Results

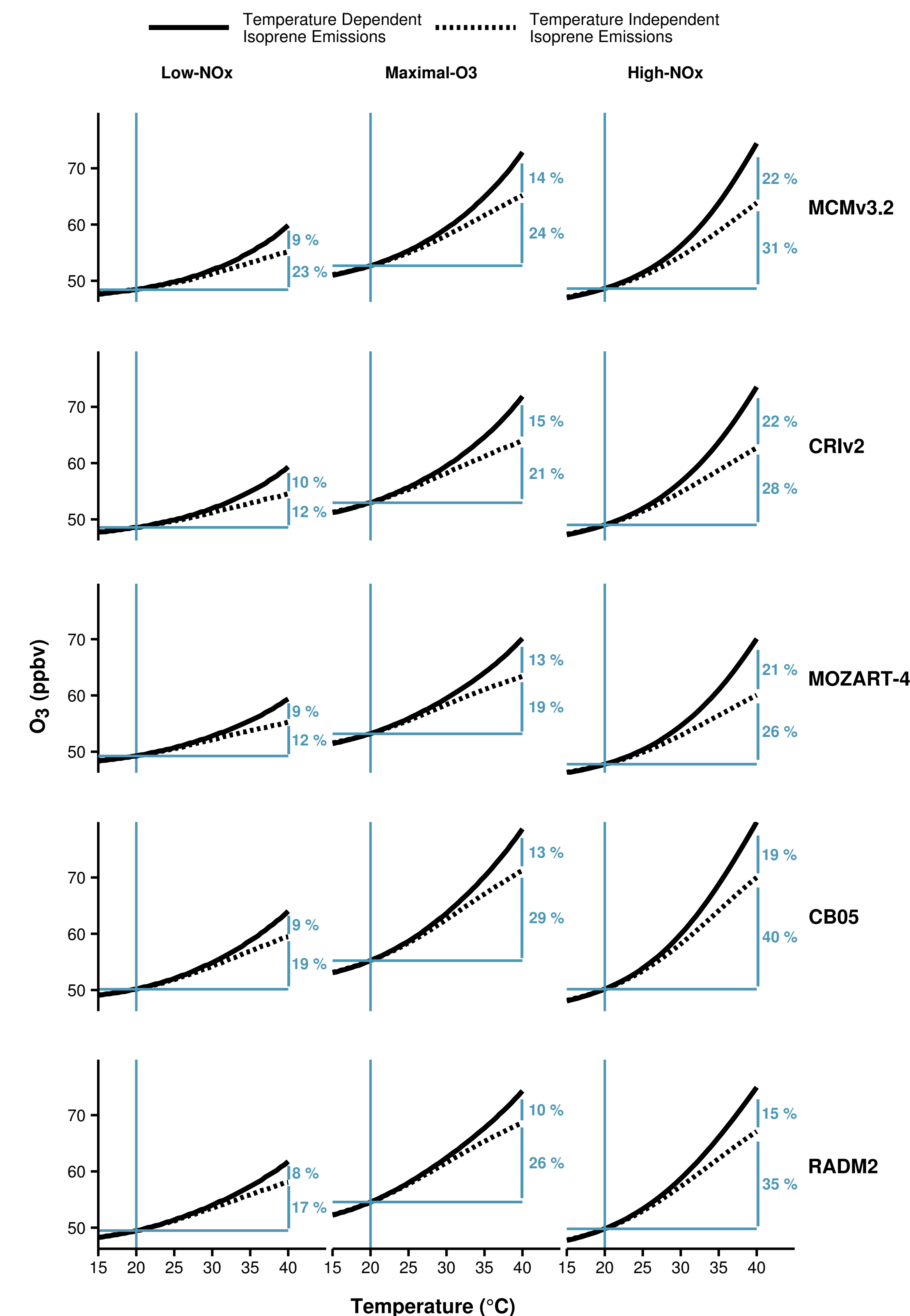
Ozone Mixing Ratios in ppbv as a Function of NO_x and Temperature



- ▶ Non-linear relationship of ozone mixing ratios with NO_x and temperature, reproduced by all chemical mechanisms.

- ▶ Higher ozone produced using RADM2 and CB05 compared to detailed chemistry of MCMv3.2

Percent Increase from 20 °C from Chemistry and Emissions



- ▶ Assigned the ozone produced to three NO_x -regimes based on $\text{H}_2\text{O}_2/\text{HNO}_3$.
- ▶ The contributions of the reactions of peroxy radicals with NO to O_x ($= \text{O}_3 + \text{NO}_2$) production budgets are determined for each NO_x -condition.
- ▶ Contributions of methyl peroxy (CH_3O_2) and acyl peroxy (CH_3CO_3) to O_x budget increases with temperature

Conclusions

- ▶ Lower NO_x levels produces the least amount of ozone regardless of the increases of emissions and chemistry. Thus, target decreases in NO_x emissions.
- ▶ All chemical mechanisms reproduce the non-linear relationship of ozone on NO_x and temperature.
- ▶ CB05 and RADM2 over-estimate the increases of ozone with temperature compared to detailed chemistry of MCMv3.2.
- ▶ The treatment of secondary chemistry in CB05 and RADM2 promotes ozone production through more aldehyde production at the expense of ketones which leads to increased levels of acyl peroxy radical (CH_3CO_3). The further degradation on CH_3CO_3 produces more ozone.

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