Institute for Advanced Sustainability Studies (IASS)

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

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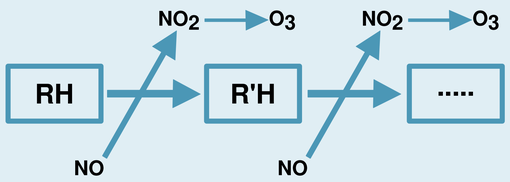
Background

- Temperature main meteorological driver of surface ozone in many areas.
- Temperature
  - increases isoprene emissions from vegetation,
  - increases reaction rates of chemical processes.
- VOC the "fuel" and NO_x the "catalyst" of ozone production.



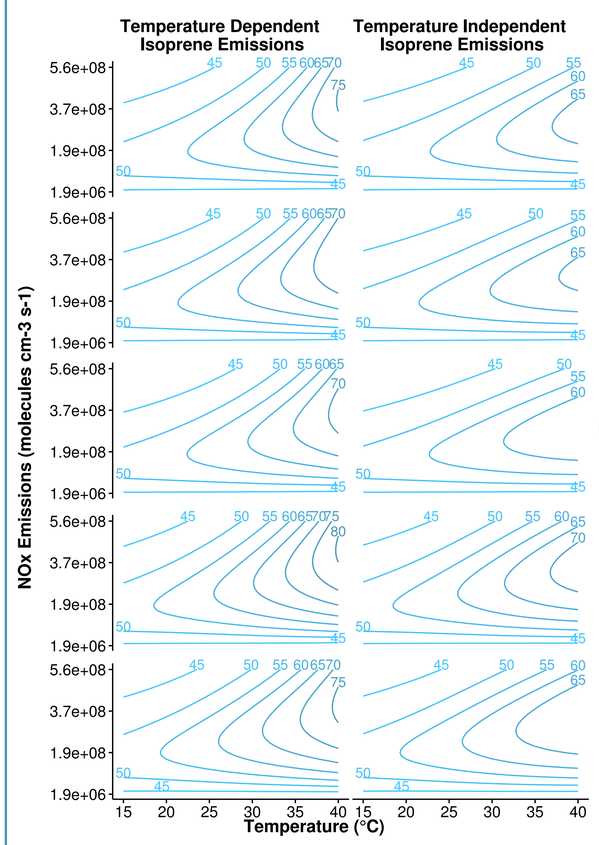
- What drives the ozone–temperature relationship? Increased isoprene emissions or chemistry?
- Can chemical mechanisms simulate the ozone–temperature relationship across NO_x gradients?

Approach

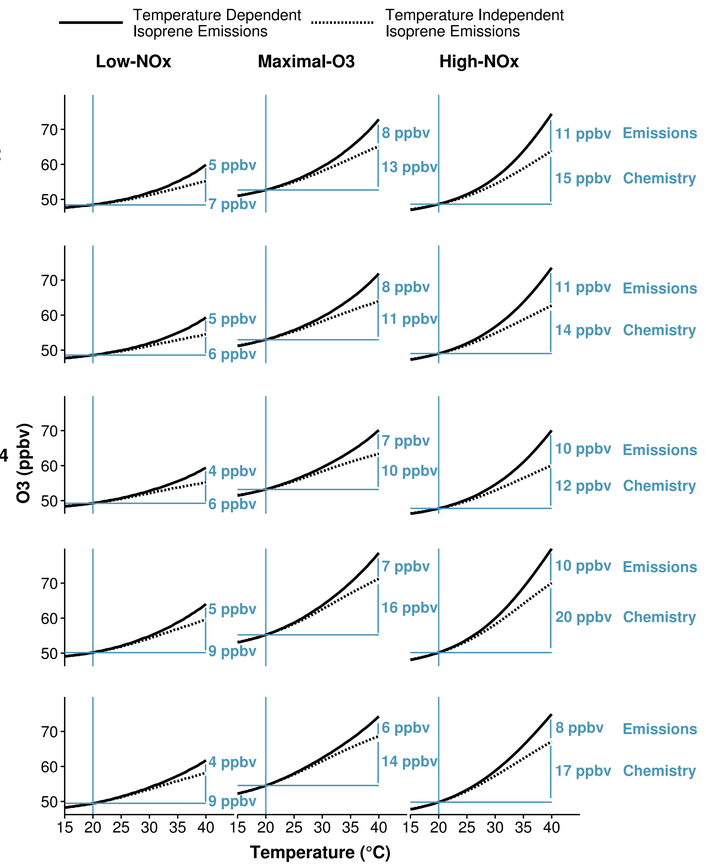
- Box model simulating urban conditions.
- Temperature dependent (MEGAN2.1) and independent isoprene emissions.
- NO_x emissions systematically varied over 15 – 40 °C.
- Repeated with chemical mechanisms: MCMv3.2, CRIv2, MOZART-4, RADM2, CB05.

Results

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



Increase in O3 mixing ratios from 20°C due to Emissions and Chemistry



- High-NO_x and temperature-dependent isoprene ⇒ highest ozone levels.
- Low-NO_x conditions has lowest ozone levels.
- Ozone levels vary non-linearly with NO_x and temperature in each chemical mechanism.
- RADM2 and CB05 produce most ozone regardless of isoprene source.

- At higher temperatures, faster reaction rates cause larger increases in ozone than higher isoprene emissions.
- High-NO_x conditions has largest increases in ozone from chemistry and emissions.
- CB05 and RADM2: more ozone from chemistry than other chemical mechanisms.

Conclusions

- Temperature-dependent chemistry responsible for most of the increase in ozone with temperature.
- High-NO_x conditions induce largest increases in ozone with temperature.
- Non-linear relationship of ozone with temperature and NO_x reproduced by all chemical mechanisms.
- Representation of chemistry in CB05 and RADM2 produces more ozone than other chemical mechanisms.

Future Work

- Compare simulated ozone–temperature to observations.
- What are the most important temperature-dependent chemical processes? PAN decomposition? Other temperature-dependent reactions?
- Why is ozone production in CB05 and RADM2 more sensitive to temperature than other mechanisms?

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