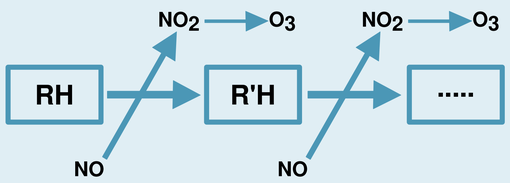
Institute for Advanced Sustainability Studies (IASS)

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

Jane Coates and Tim Butler

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.



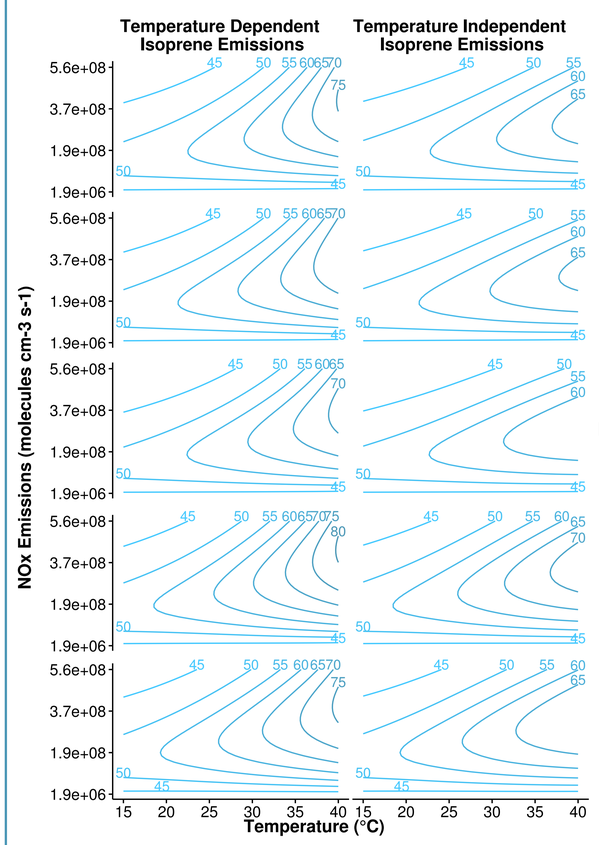
- What drives the ozone–temperature relationship? Increased isoprene emissions or chemistry?
- Can chemical mechanisms simulate the ozone–temperature relationship across NO_x gradients?

Approach

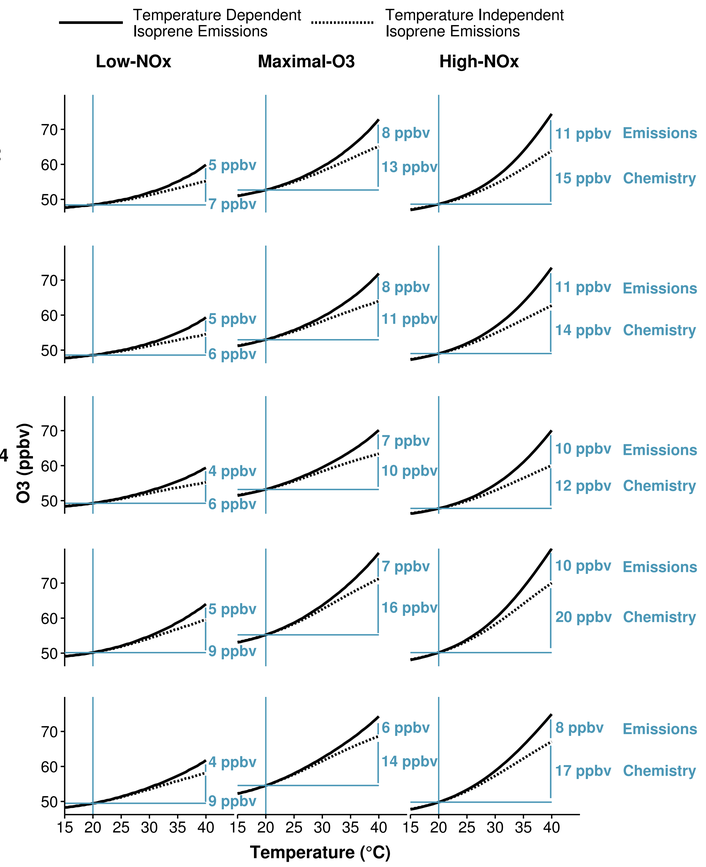
- Box model simulating Benelux region.
- Temperature dependent and independent isoprene emissions.
- NO_x emissions systematically varied over 15 – 40 °C.
- Repeated with chemical mechanisms: MCMv3.2, CRIv2, MOZART-4, RADM2, CB05.

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.

- Faster reaction rates cause larger increase in ozone than higher isoprene emissions.
- High-NO_x conditions has largest increases in ozone from chemistry and emissions.
- Increased isoprene emissions in CB05 and RADM2 produces less ozone than other chemical mechanisms.

Conclusions

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

Future Work

- Compare simulated ozone–temperature to observations.
- What are the most important temperature-dependent chemical processes? PAN decomposition? Increased radical production?
- Why do CB05 and RADM2 produce more ozone than other mechanisms?

The IASS is sponsored by

SPONSORED BY THE
Federal Ministry of Education and Research
FONA Research for Sustainable Development
BMBF
LAND BRANDENBURG
Ministerium für Wissenschaft, Forschung und Kultur