Institute for Advanced Sustainability Studies (IASS)

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

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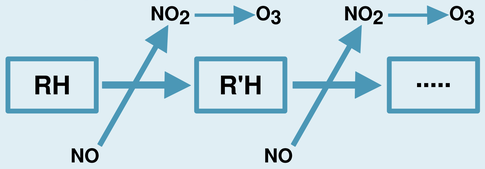
Background



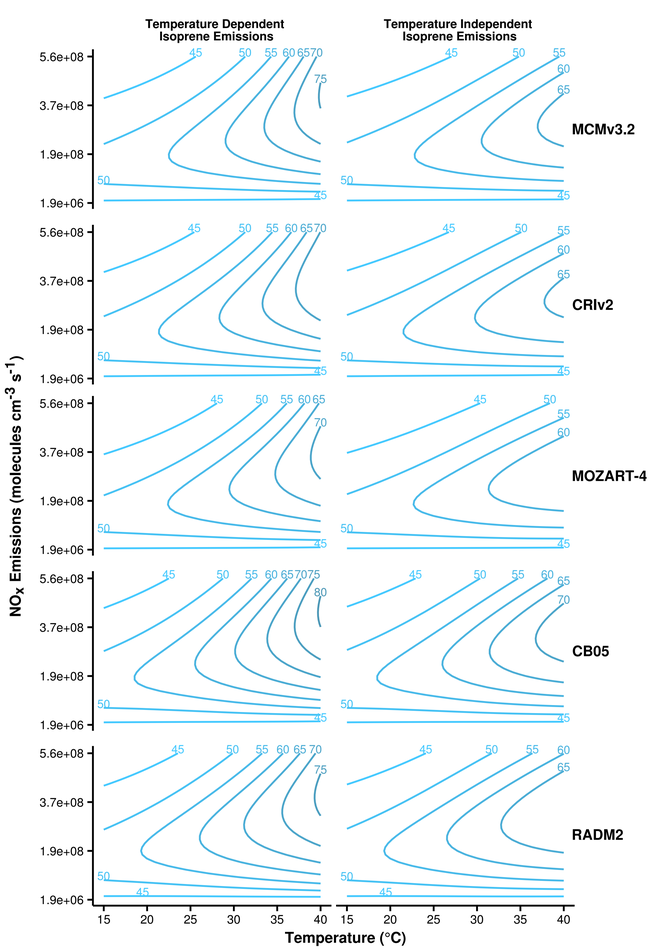
- Ozone is produced from photochemistry of emitted VOC and NO_x, VOC is the "fuel" and NO_x the "catalyst".
- Climate change will increase surface temperatures.
- Temperature drives surface ozone in many areas.
- Temperature influences ozone production by
  - increasing BVOC emissions from vegetation,
  - increasing reaction rates atmospheric chemistry.
- Is increased BVOC emissions or increased chemistry more important for increasing ozone with temperature?
- Do chemical mechanisms used in models reproduce the relationship between ozone and temperature across NO_x gradients?

Approach

- Idealised box model simulating central europe (Benelux).
- Systematic variations in NOx over temperature range (15 – 40 °C).
- Simulations repeated using temperature dependent and independent source of isoprene emissions.
- All simulations repeated using chemical mechanisms that represent atmospheric chemistry at different scales: Point - MCMv3.2; regional - CRIv2, MOZART-4, CB05, RADM2.

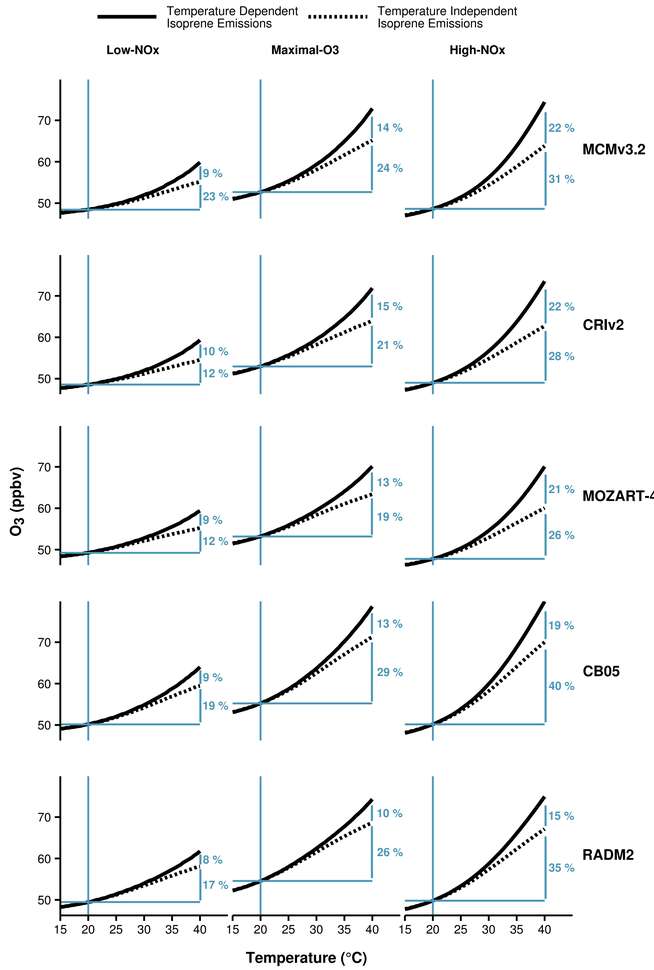
Results

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.
- Increased ozone when including temperature dependent source of isoprene, especially at high-NO_x.

Percent Increase from 20°C from Chemistry and Emissions



- Contributions of methyl peroxy (CH_3O_2) and acyl peroxy (CH_3CO_3) to O_x budget increases with temperature.
- CH_3CO_3 is a precursor of CH_3O_2 which in turn is a precursor of HO_2. Thus increased source of a precursor of CH_3CO_3 - acetaldehyde - leads to higher ozone production.
- Acetaldehyde is an important carbonyl product, especially during isoprene degradation, and in

Conclusions

- Lower NOx 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.

Future Work

- Compare results to ERA-Interim data.

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