



Tropospheric Ozone Production Pathways with Detailed Chemical Mechanisms

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17th March 2015

Introduction and Motivation

Previous Meeting Re-cap

Comparison of O_x Production in Chemical Mechanisms

Impact of Solvent Speciations on O_3

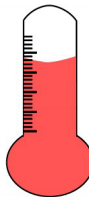
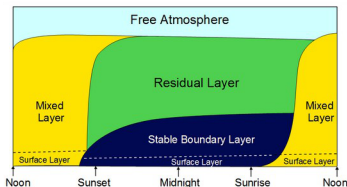
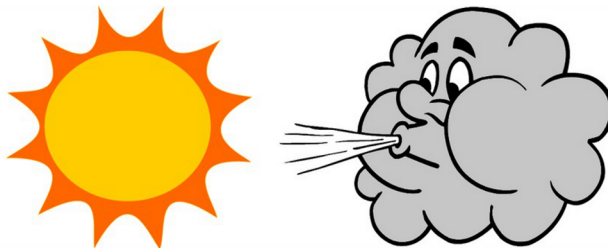
Other Contributions

Future Pathways

Tropospheric Ozone



Meteorology Affects O₃ Formation



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Other Contributions

Future Pathways

Re-Cap of Previous Meeting



- ▶ Include CB05 in mechanism comparison study.
- ▶ Submit mechanism comparison paper to ACP.
- ▶ O_x production under different conditions:
use all mechanisms or just a subset?
- ▶ Use realistic conditions from regional model.
- ▶ Compare VOC substitution techniques using WRF-Chem with Katie.

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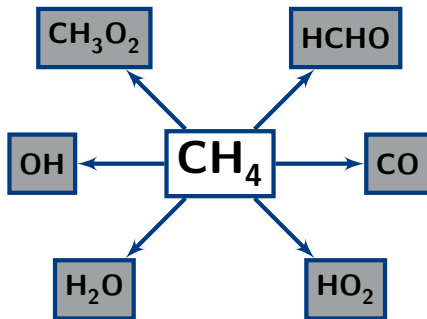
Other Contributions

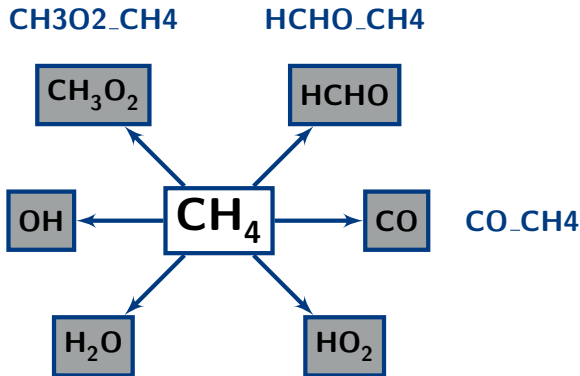
Future Pathways

How is O_x production affected by the differing simplification techniques used in different chemical mechanisms?

Chemical Mechanism	Lumping Approach	Reference
MCM v3.2	No lumping	[http://mcm.leeds.ac.uk/MCM/]
MCM v3.1	No lumping	[Saunders et al., ACP, 2003] [Jenkin et al., ACP, 2003]
CRI v2	Lumped intermediates	[Jenkin et al., AE, 2008]
MOZART-4	Lumped molecule	[Emmons et al., GMD, 2010]
RADM2	Lumped molecule	[Stockwell et al., JGR, 1990]
RACM	Lumped molecule	[Stockwell et al., JGR, 1997]
RACM2	Lumped molecule	[Goliff et al., AE, 2013]
CBM-IV	Lumped structure	[Gery et al., JGR, 1989]
CB05	Lumped structure	[Yarwood et al., EPA report, 2005]

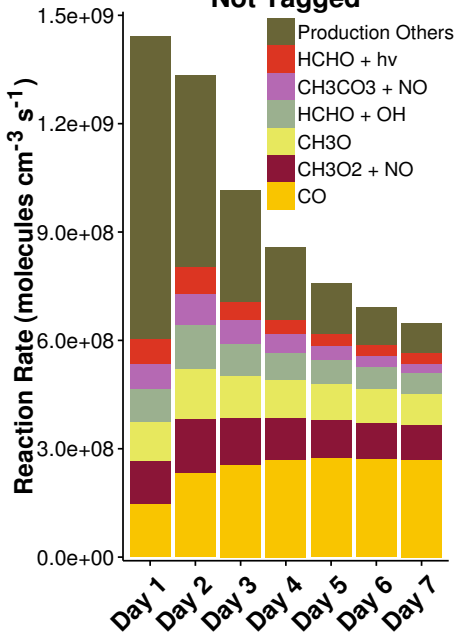
- ▶ MECCA boxmodel over Los Angeles, under equinoctical conditions over 7 days.
- ▶ Initial NMVOC typical of urban environments.
- ▶ Same NMVOC emissions and reactive carbon in each model run.
- ▶ NO source tuned for maximum O_3 production.
- ▶ Mechanisms tagged for each NMVOC.



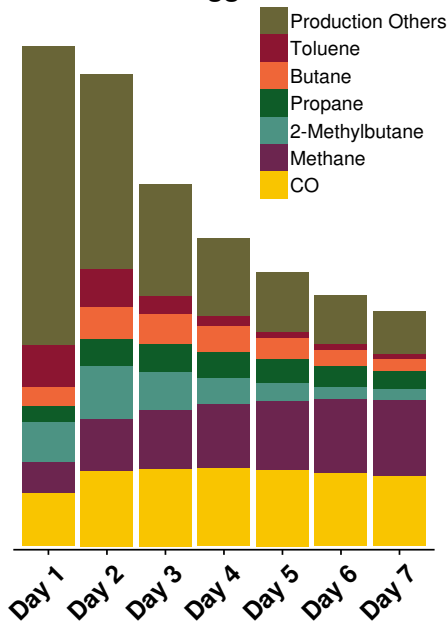


O_x Production Budgets

Not Tagged



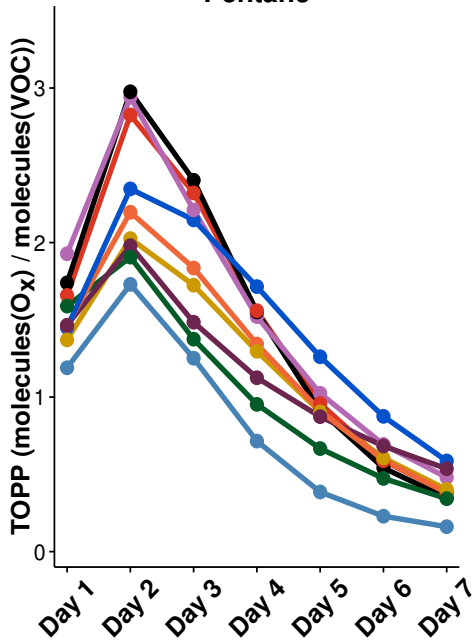
Tagged



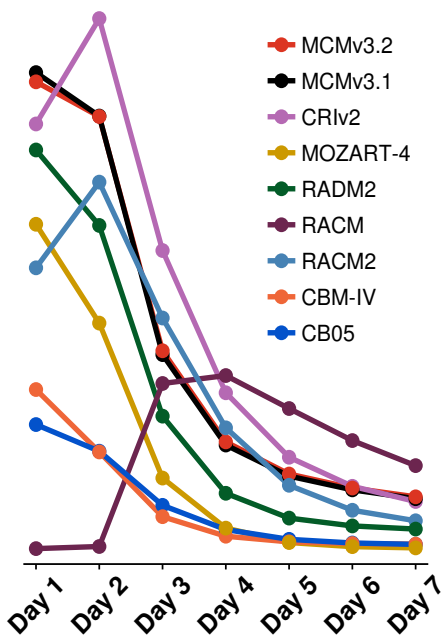
- ▶ Attribute daily O_x production to each NMVOC.
- ▶ Sum daily O_x production from each NMVOC.
- ▶ Normalise by total emissions of the NMVOC on day 1.

Daily O_x Production

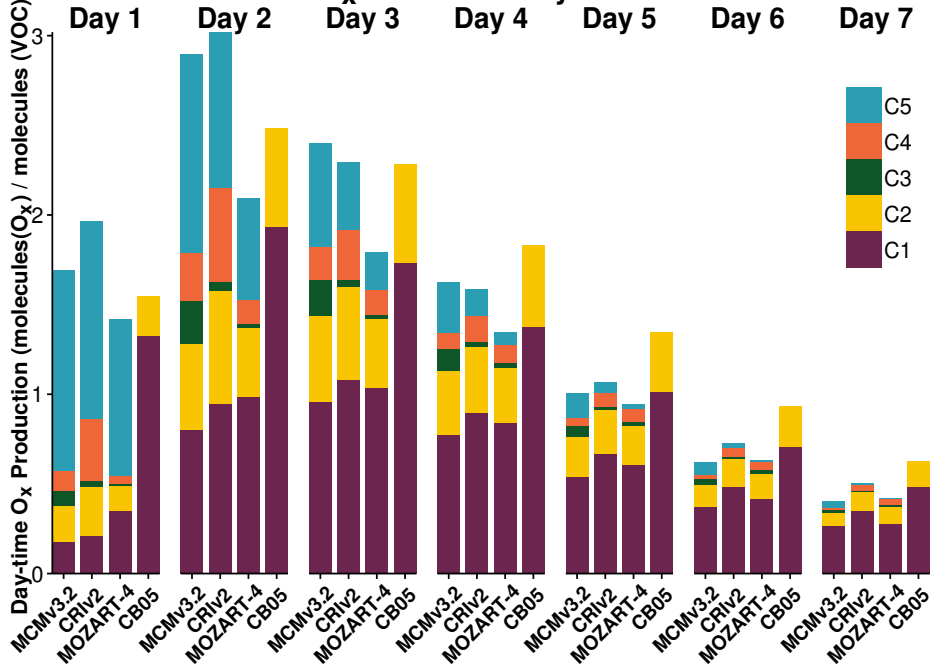
Pentane



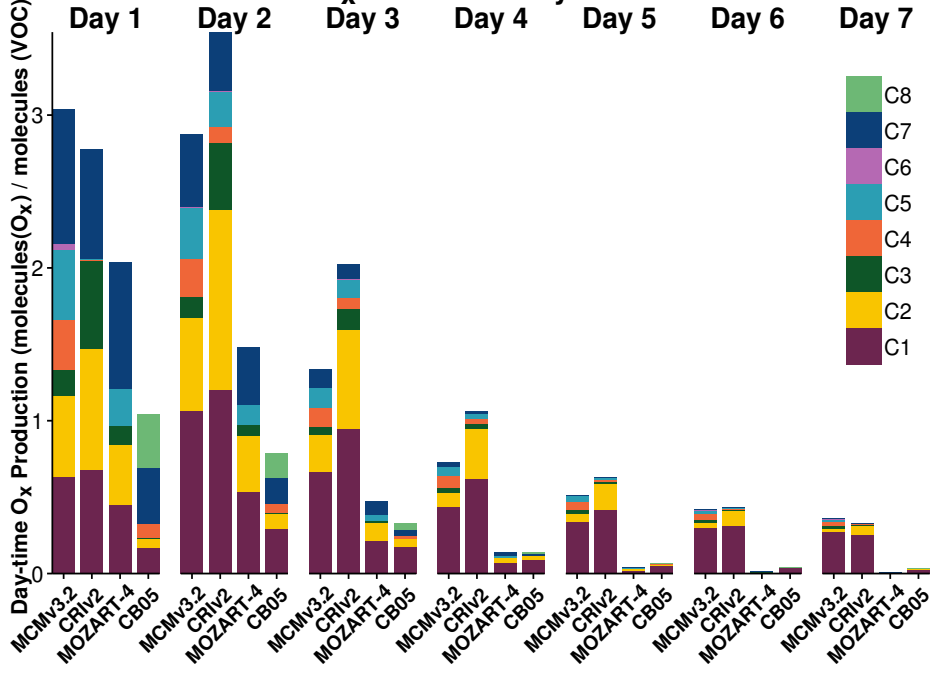
Toluene



Pentane : O_x Production by Carbon Number

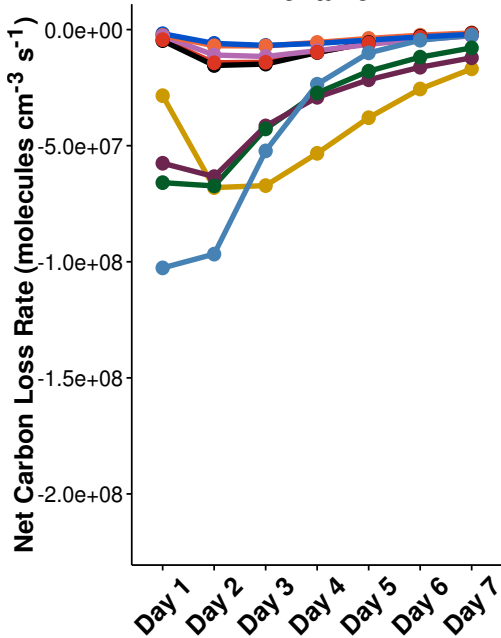


Toluene : O_x Production by Carbon Number

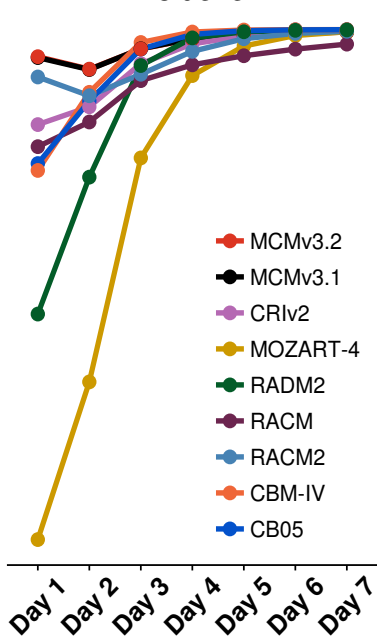


Loss Rates of Carbon

Pentane



Toluene



Paper Status



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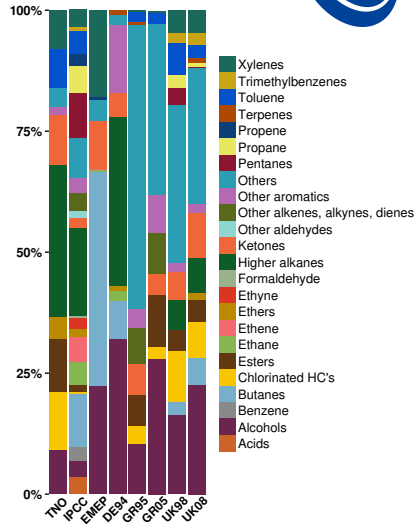
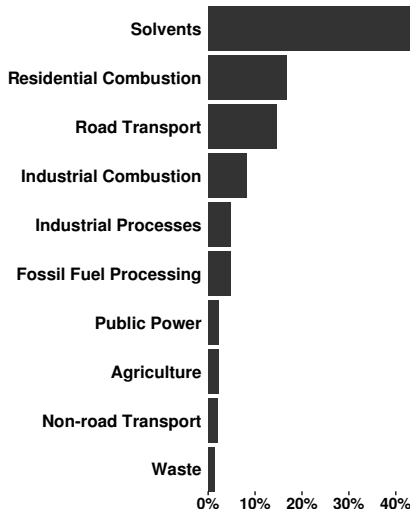
Impact of Solvent Speciations on O_3

Other Contributions

Future Pathways

How does VOC speciation affect
O₃ concentrations in models?

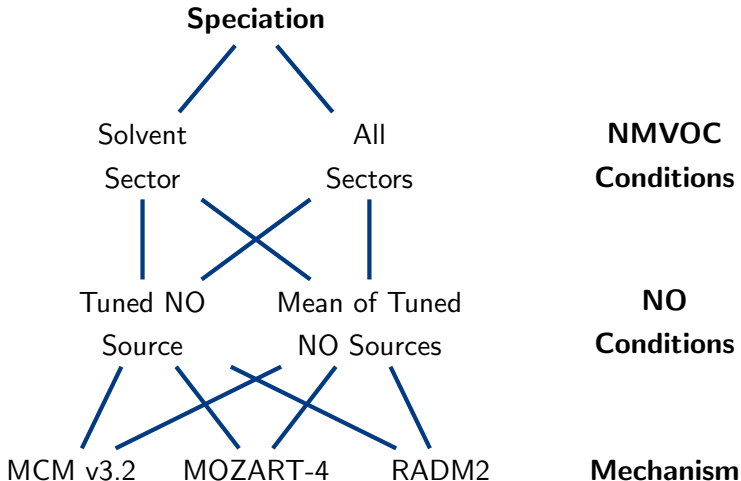
Motivation



Compared Solvent Speciations

Speciation	Reference
TNO	[Stockwell et al., JGR, 1997]
IPCC	[Stockwell et al., JGR, 1990]
EMEP	[Saunders et al., ACP, 2003]
DE94	[http://mcm.leeds.ac.uk/MCM/]
GR95	[Emmons et al., GMD, 2010]
GR05	[Jenkin et al., AE, 2008]
UK98	[Yarwood et al., EPA report, 2005]
UK08	[Goliff et al., AE, 2013]

- ▶ MECCA boxmodel, equinoctical conditions over 7 days.
- ▶ Idealised urban area of 1000 km².
- ▶ Total NMVOC emissions of 1000 ton/day
[Warnecke et al., JGR, 2007].
- ▶ NMVOC emissions constant until noon of day 1.



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Other Contributions

Future Pathways

- ▶ Presentations and Posters
 - ▶ Poster and presentation at PhD Conference on Earth System Science, Mar 2014.
 - ▶ Poster at IASS Evaluation, May 2014.
 - ▶ Poster at Our Climate Our Future (REKLIM) Conference, Oct 2014.
 - ▶ Presentation at OH Reactivity Specialists Uniting Meeting (ORSUM), Oct 2014.
- ▶ Courses
 - ▶ Atmospheric Science in Context of Global Change at Potsdam Universität by Prof. Mark Lawrence, Oct 2013 – Jan 2014.
 - ▶ Presenting Data and Information by Edward Tufte, Feb 2015.

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Other Contributions

Future Pathways

- ▶ Conclude chemical mechanism study.
 - ▶ Include SAPRC-11?
- ▶ Publish chemical mechanism study results.
 - ▶ Split into two papers?

- ▶ Different meteorological parameters.
 - ▶ Temperature.
 - ▶ Amount of sunlight.
- ▶ Different NO_x concentrations.
- ▶ Calculate indirect effects of VOC degradation.
- ▶ TOPP values in more realistic atmospheric conditions.
- ▶ Improve lumping of emitted VOC species in models.