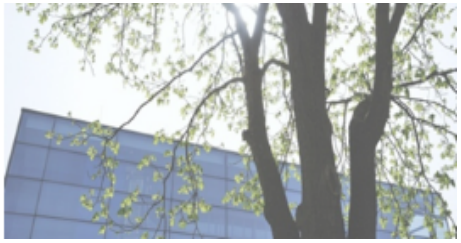



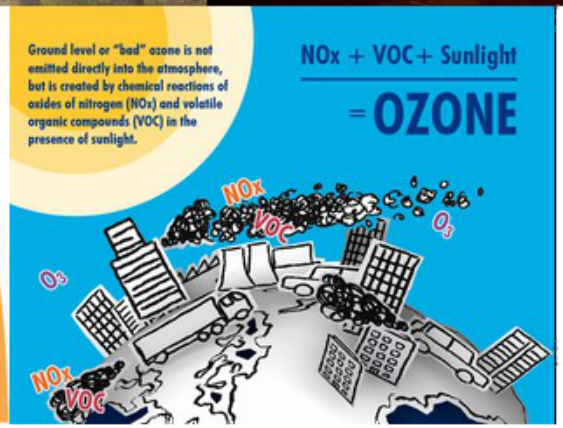
Tropospheric Ozone Production Pathways with Detailed Chemical Mechanisms

Jane Coates

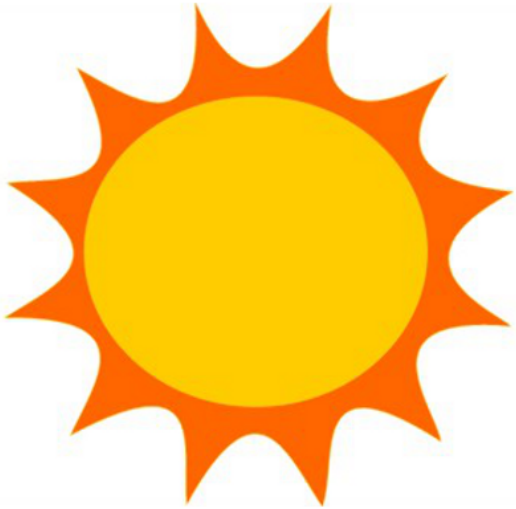
17th March 2015

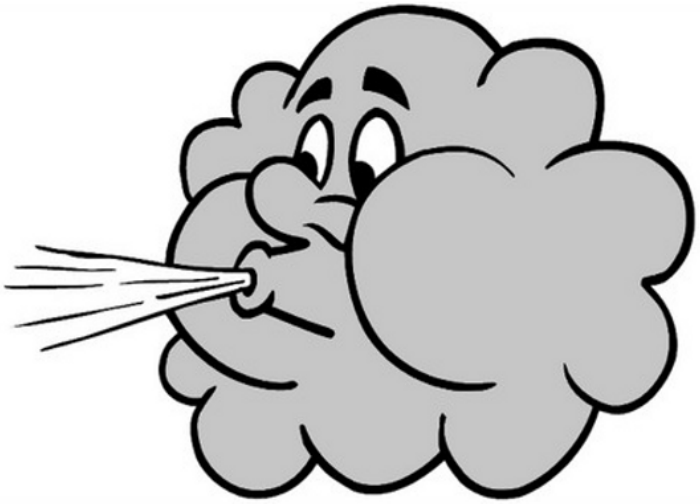
Outline

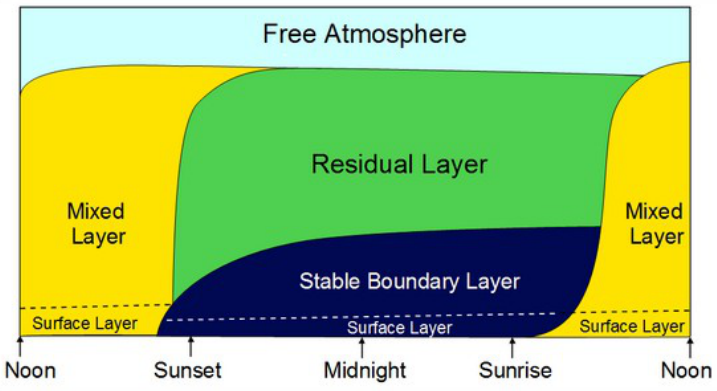
Tropospheric Ozone

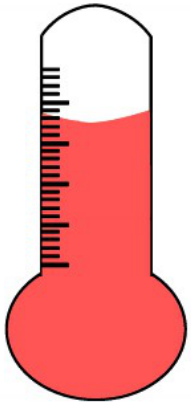


Meteorological impacts on O_3 Production

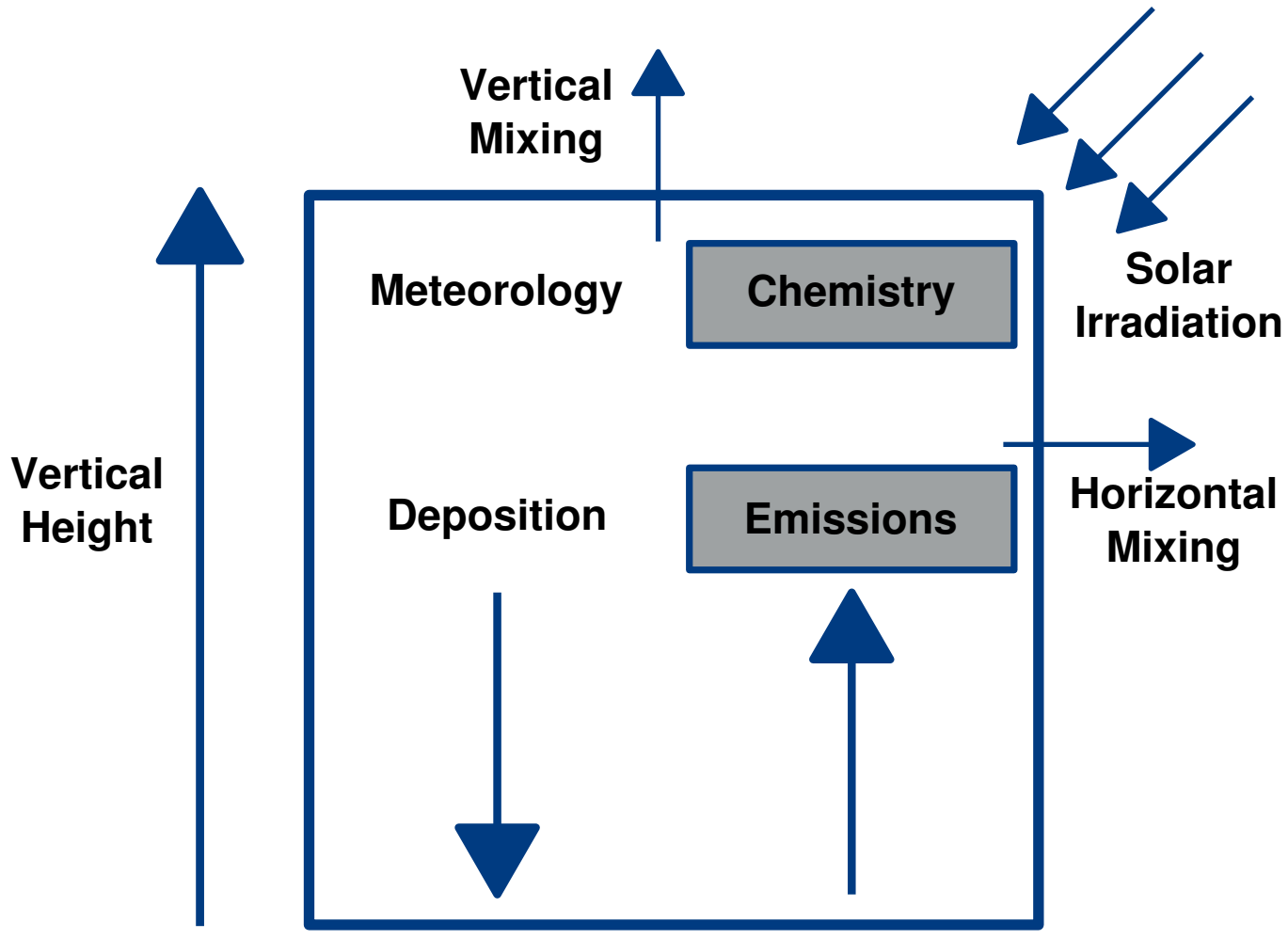








Modelling


Vertical
Mixing
Meteorology
Chemistry
Solar
Irradiation
Vertical
Height
Deposition
Emissions
Horizontal
Mixing

Outline

Action Points from Last Meeting

- Include CB05 in mechanism comparison study. ✓
- Submit mechanism comparison paper to ACP.
- O_3 concentrations using different solvent sector emissions. ✓
- O_x production under different conditions:
  use all mechanisms or a subset?
- Use realistic conditions from regional model.

Outline

Main Research Question

How do the simplification techniques used in different chemical mechanisms affect O_x production?

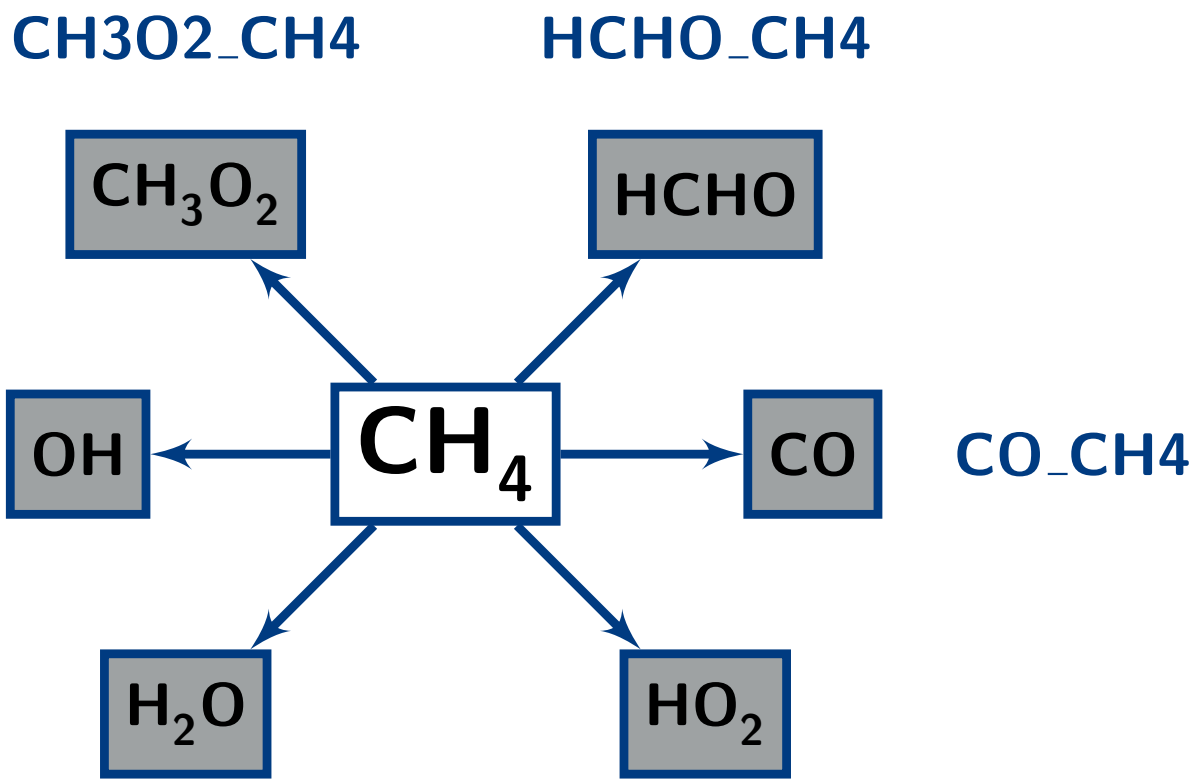
Chemical Mechanisms

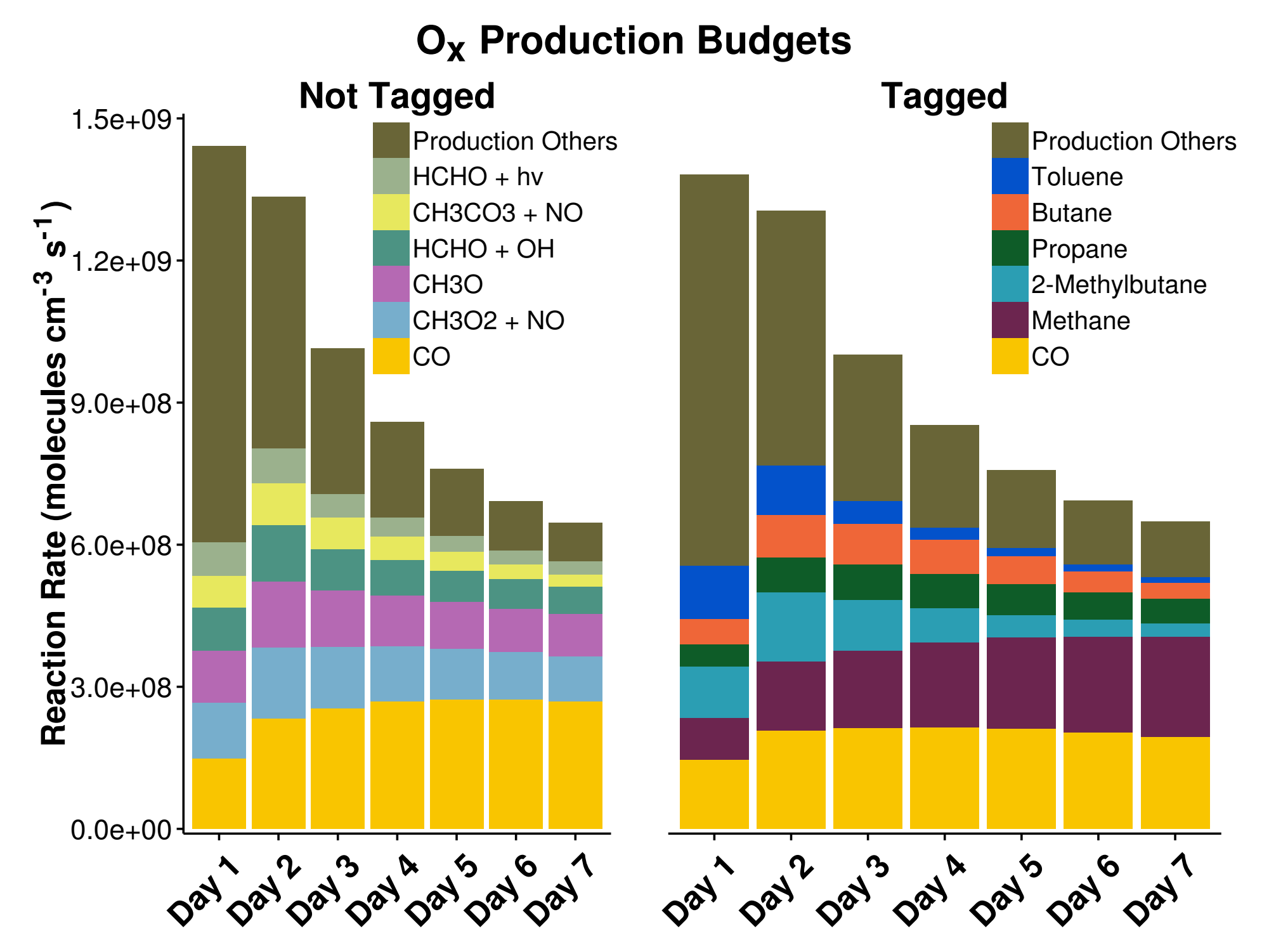
Chemical Mechanism	Lumping Approach	Reference
MCM v3.2	No lumping	[http://mcm.leeds.ac.uk/MCM/]
MCM v3.1	No lumping	[Saunders et al., ACP, 2003] [Jenkin et al., ACP, 2003]
CRI v2	Lumped intermediates	[Jenkin et al., AE, 2008]
MOZART-4	Lumped molecule	[Emmons et al., GMD, 2010]
RADM2	Lumped molecule	[Stockwell 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]

Boxmodel Setup

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

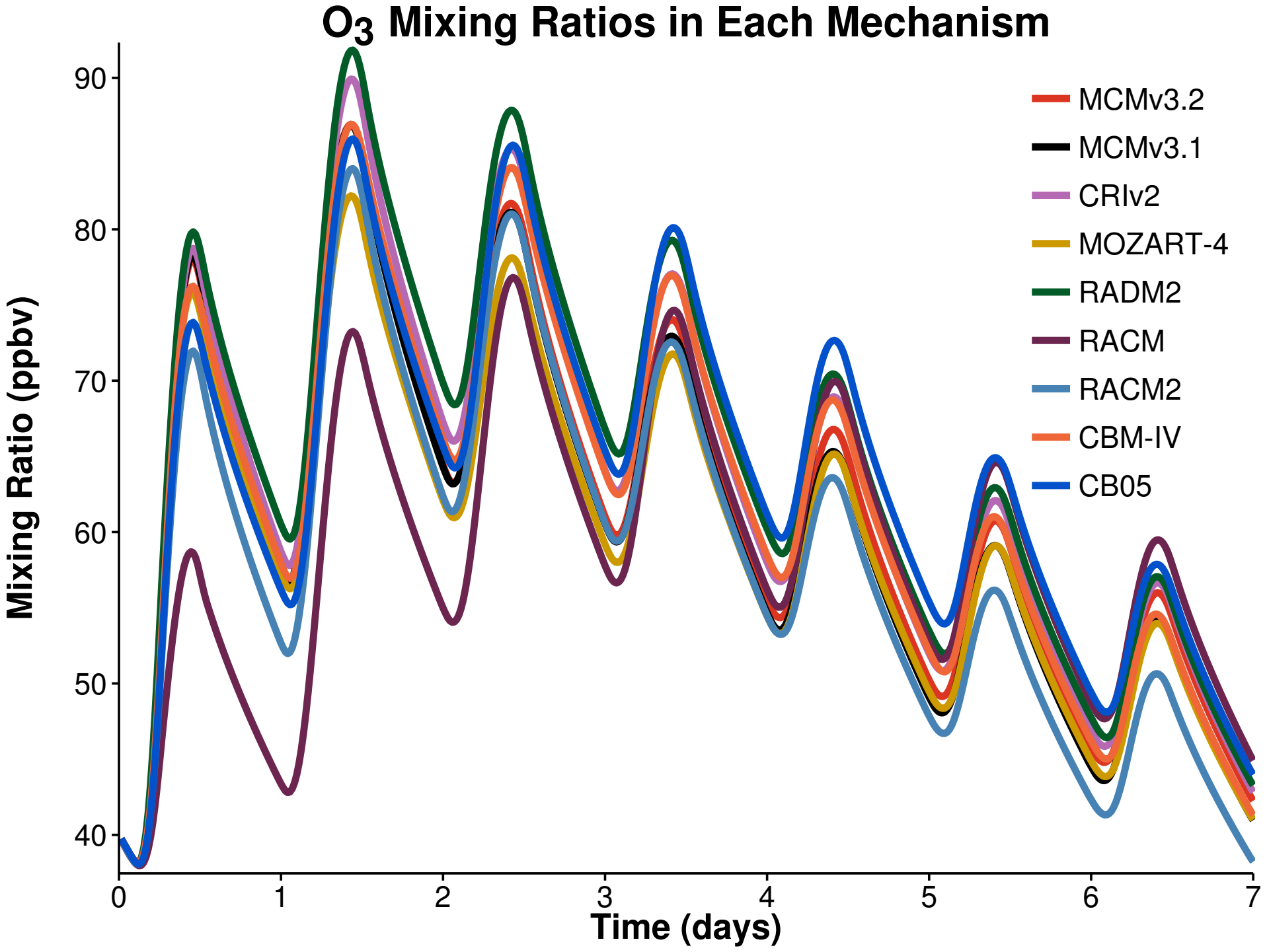
Organic Degradation Product Tagging

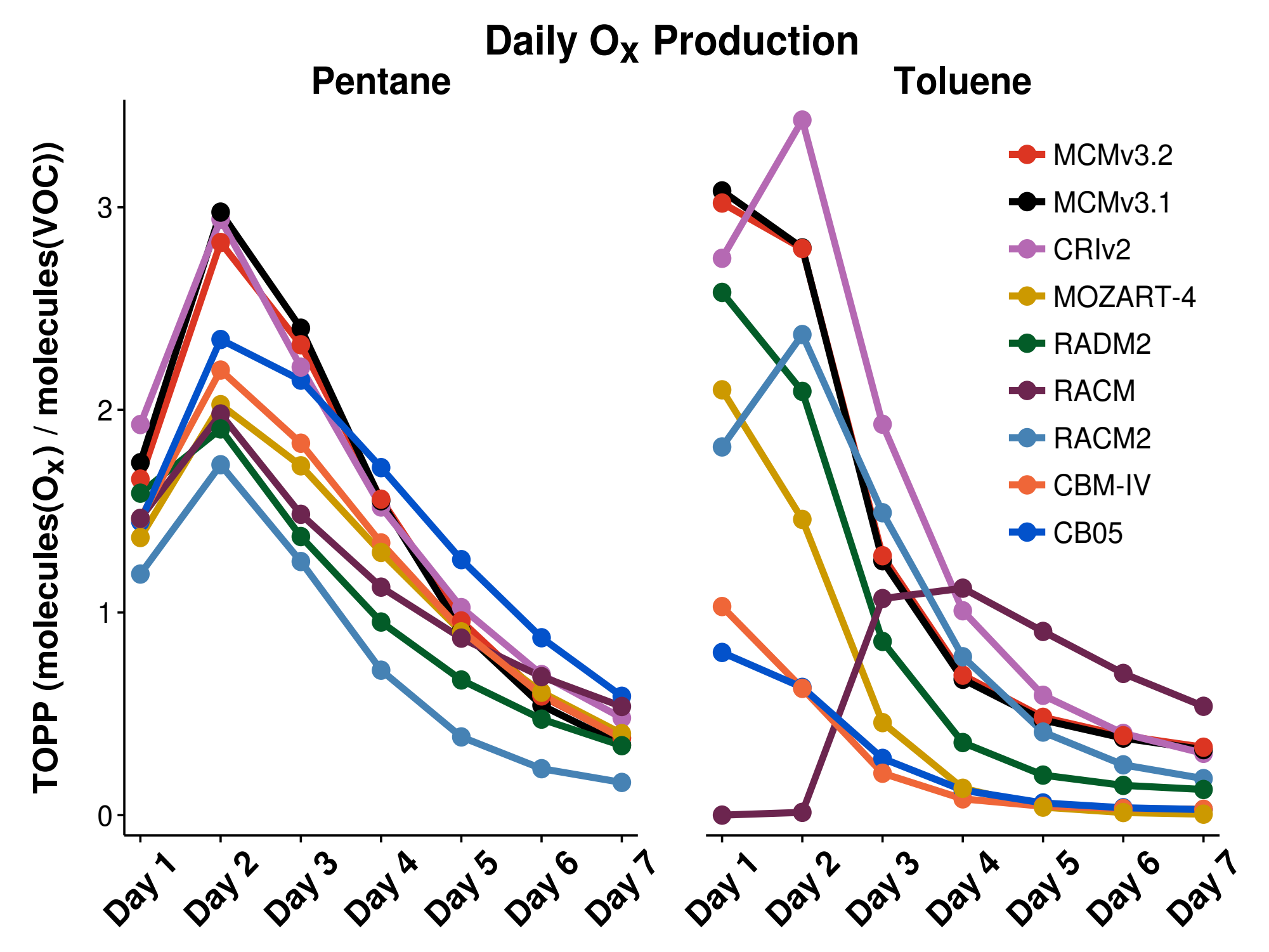


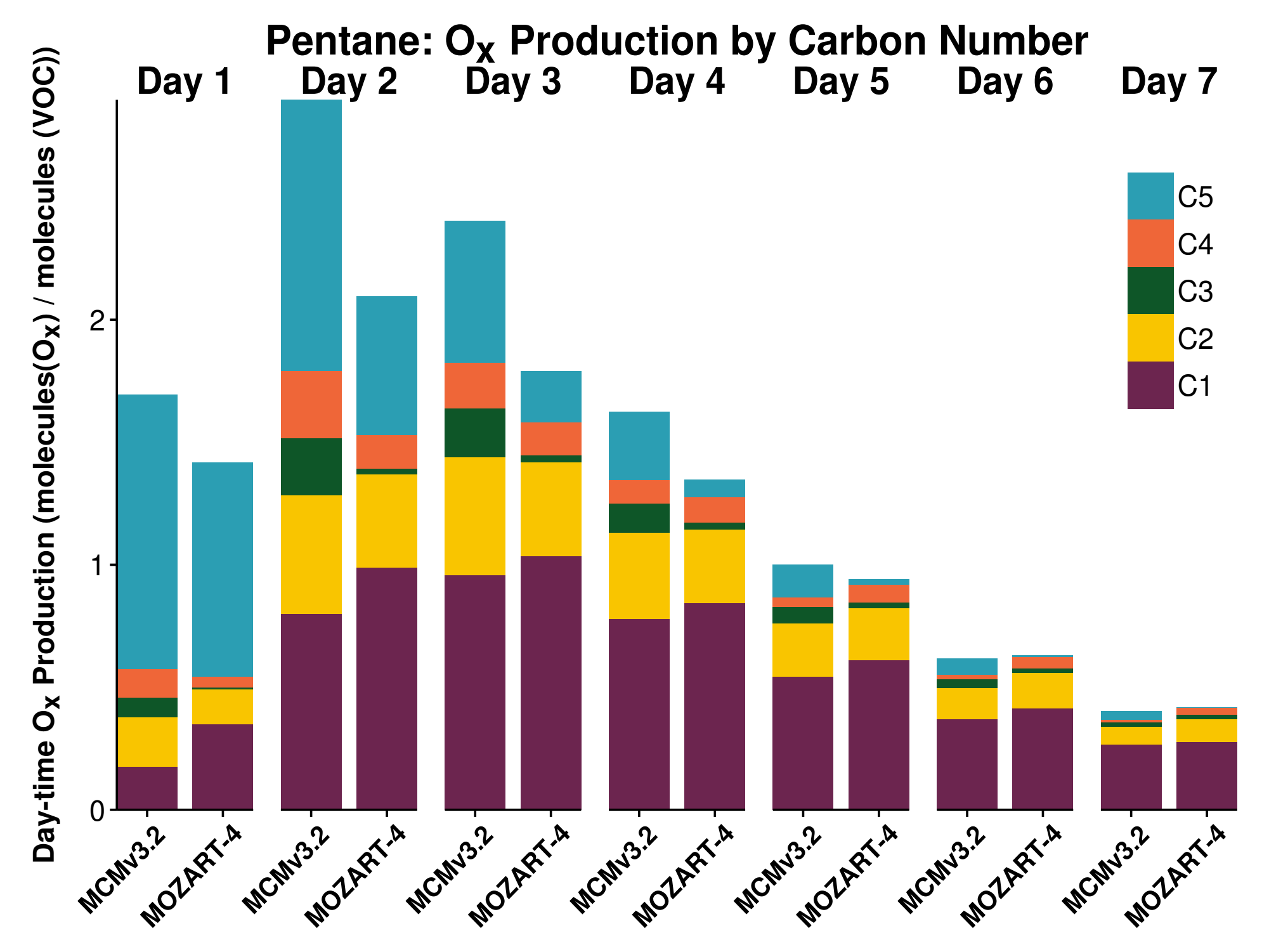

O_x Production Budgets
Not Tagged
Tagged
Reaction Rate (molecules cm^{-3} s^{-1})
1.5e+09
1.2e+09
9.0e+08
6.0e+08
3.0e+08
0.0e+00
Production Others
HCHO + hv
CH3CO3 + NO
HCHO + OH
CH3O
CH3O2 + NO
CO
Production Others
Toluene
Butane
Propane
2-Methylbutane
Methane
CO
Day 1
Day 2
Day 3
Day 4
Day 5
Day 6
Day 7

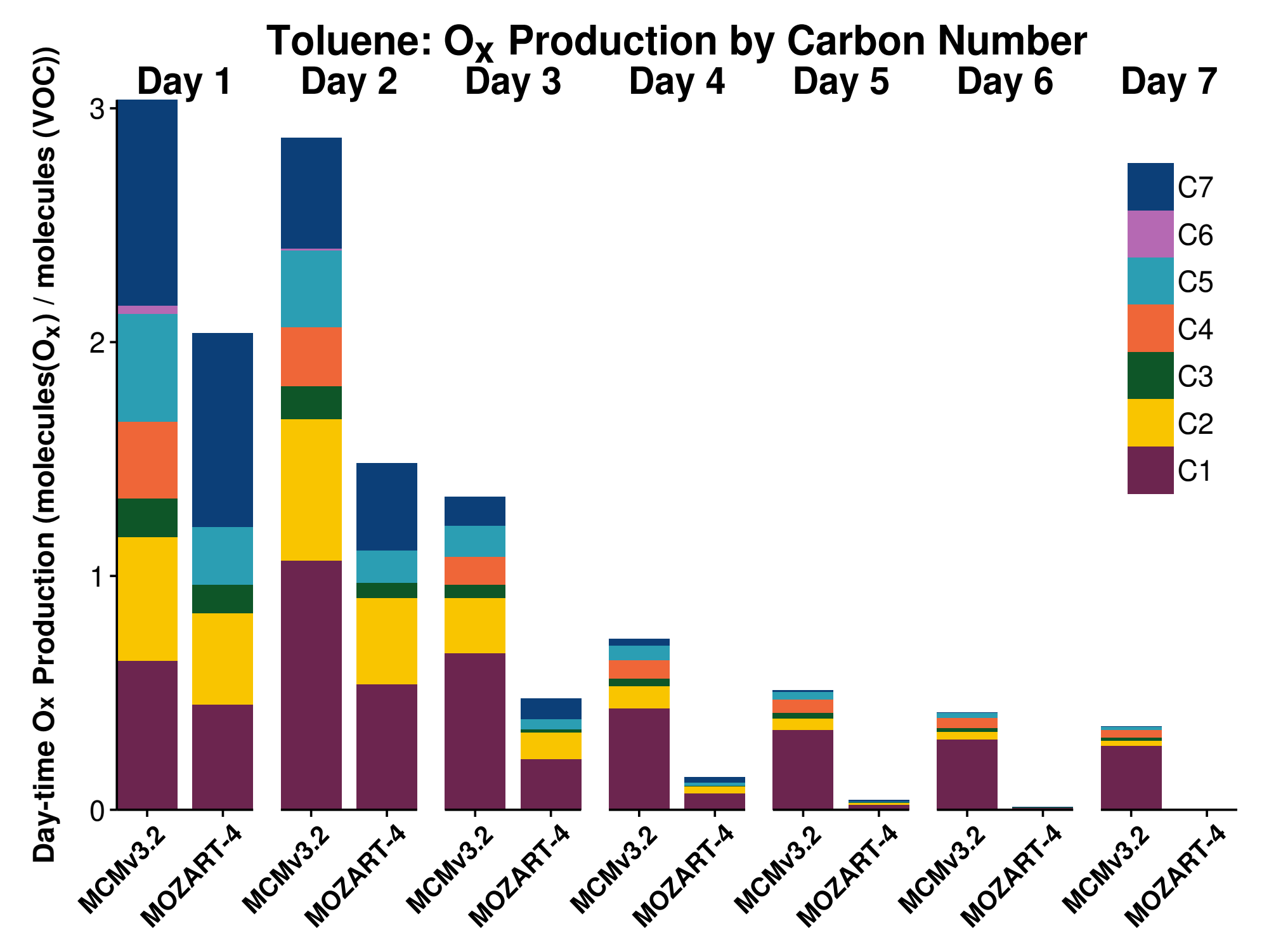
TOPP Calculation

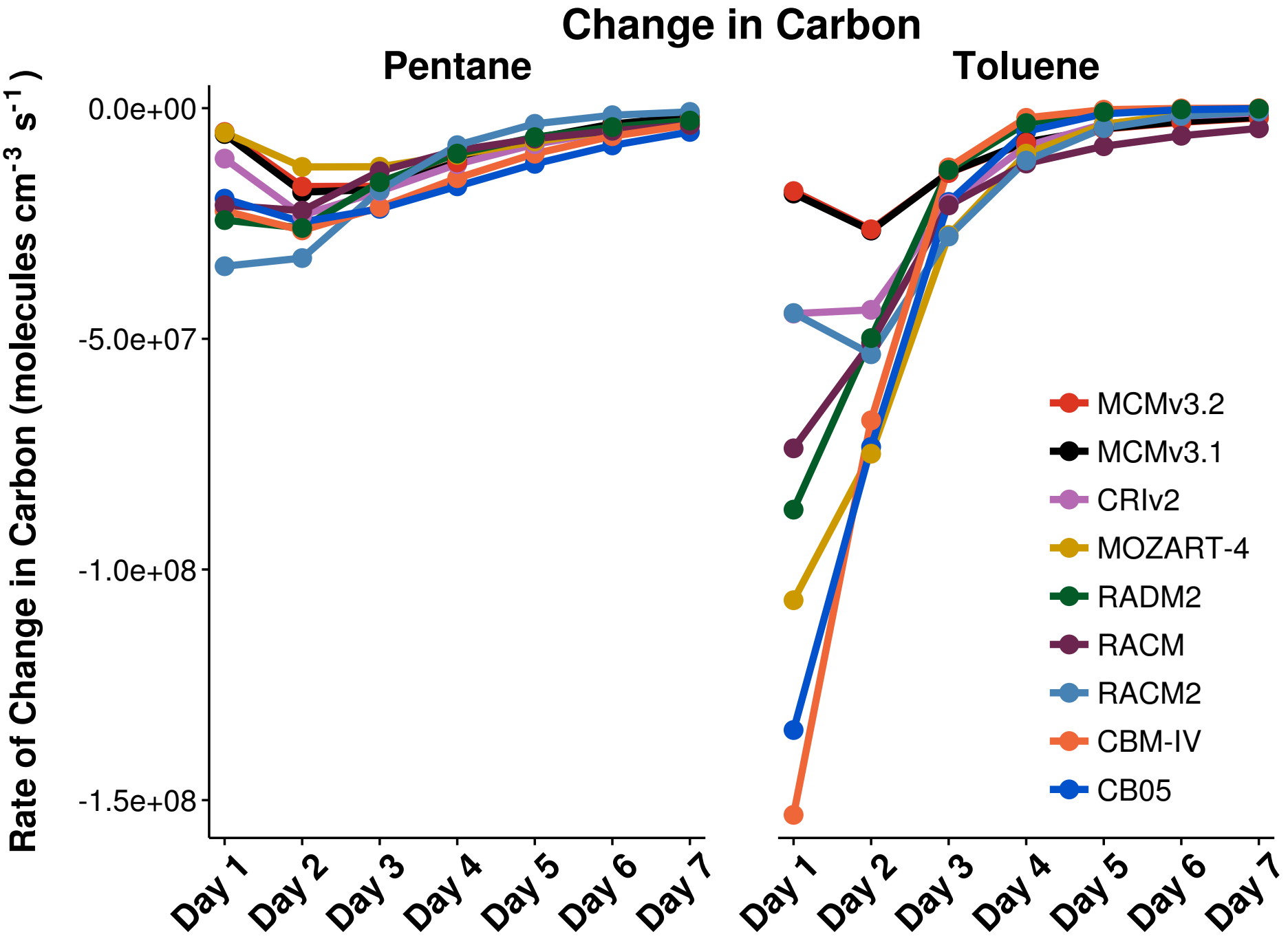
- Attribute daily O_x production to each NMVOC.
- Sum daily O_x production from each NMVOC.
- Normalise by total emissions of the NMVOC on day 1.

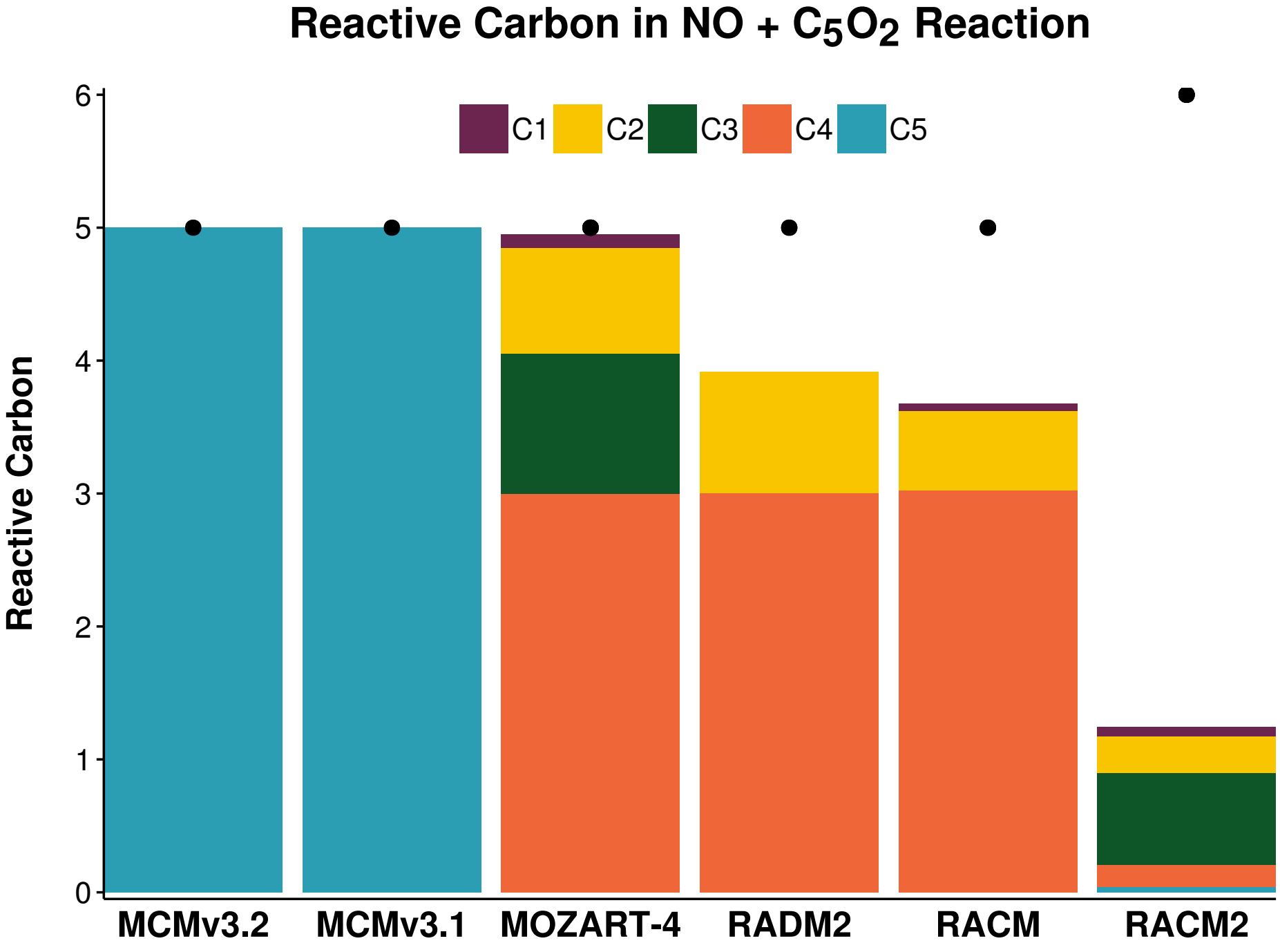

O_3 Mixing Ratios in Each Mechanism
Mixing Ratio (ppbv)
90
80
70
60
50
40
0
1
2
3
4
5
6
7
Time (days)
MCMv3.2
MCMv3.1
CRIv2
MOZART-4
RADM2
RACM
RACM2
CBM-IV
CB05


Daily O_x Production
Pentane
Toluene
TOPP (molecules(O_x) / molecules(VOC))
0
1
2
3
Day 1
Day 2
Day 3
Day 4
Day 5
Day 6
Day 7
MCMv3.2
MCMv3.1
CRIv2
MOZART-4
RADM2
RACM
RACM2
CBM-IV
CB05

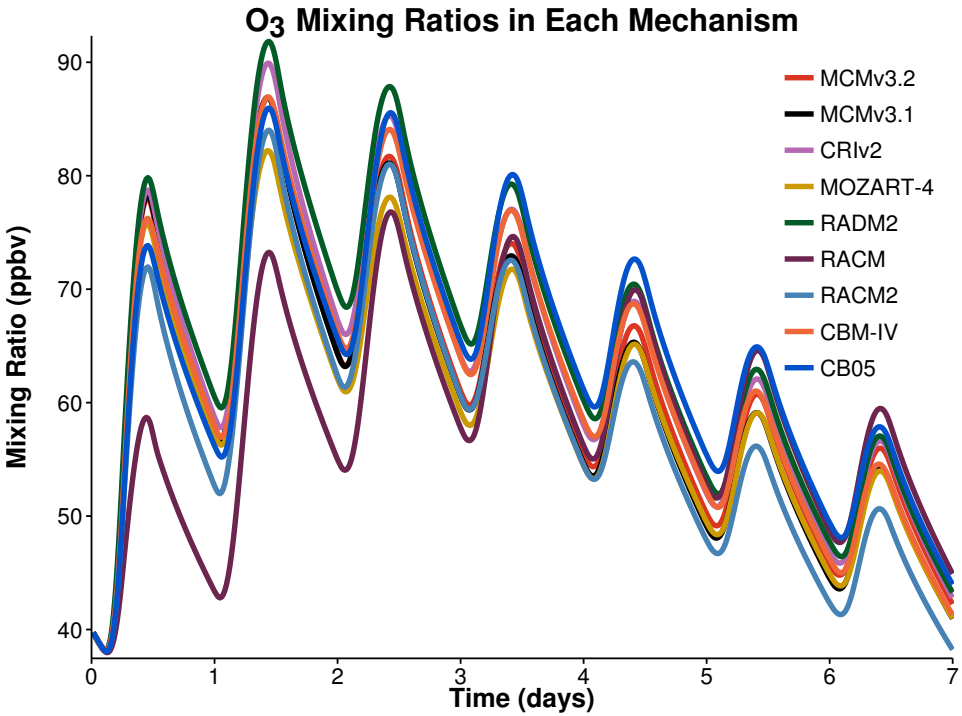

Pentane: O_X Production by Carbon Number
Day 1
Day 2
Day 3
Day 4
Day 5
Day 6
Day 7
Day-time O_X Production (molecules(O_X) / molecules (VOC))
0
1
2
C5
C4
C3
C2
C1
MCMv3.2
MOZART-4


Toluene: O_x Production by Carbon Number
Day 1
Day 2
Day 3
Day 4
Day 5
Day 6
Day 7
Day-time Ox Production (molecules(O_x) / molecules (VOC))
0
1
2
3
C7
C6
C5
C4
C3
C2
C1
MCMv3.2
MOZART-4


Change in Carbon
Pentane
Toluene
Rate of Change in Carbon (molecules cm-3 s-1)
0.0e+00
-5.0e+07
-1.0e+08
-1.5e+08
Day 1
Day 2
Day 3
Day 4
Day 5
Day 6
Day 7
MCMv3.2
MCMv3.1
CRIv2
MOZART-4
RADM2
RACM
RACM2
CBM-IV
CB05


Reactive Carbon in NO + C5O2 Reaction
C1
C2
C3
C4
C5
Reactive Carbon
0
1
2
3
4
5
6
MCMv3.2
MCMv3.1
MOZART-4
RADM2
RACM
RACM2

Conclusions



- Reduced mechanisms break down many VOC faster than MCM.
- Many VOC produce similar Ox to MCM on first day, but not subsequent days.

Paper Status

- Advanced draft of paper sent for internal review.
- Discuss draft as part of this meeting.

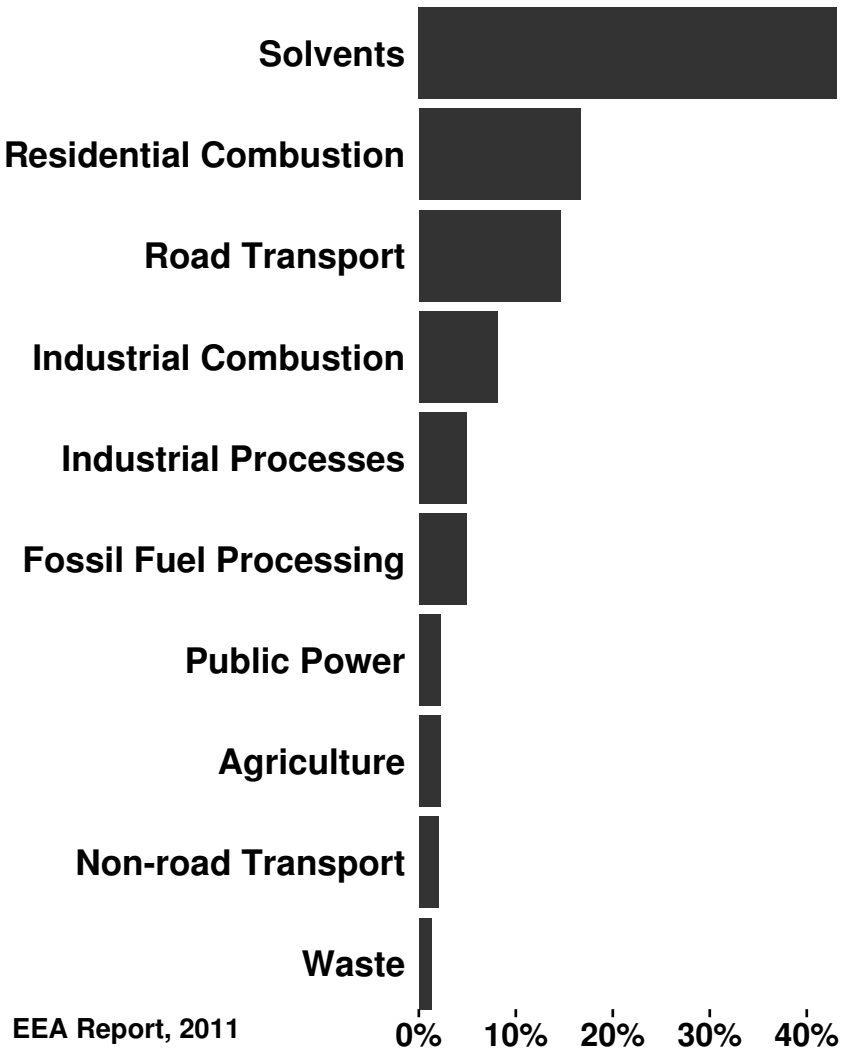
Outline

Main Research Question

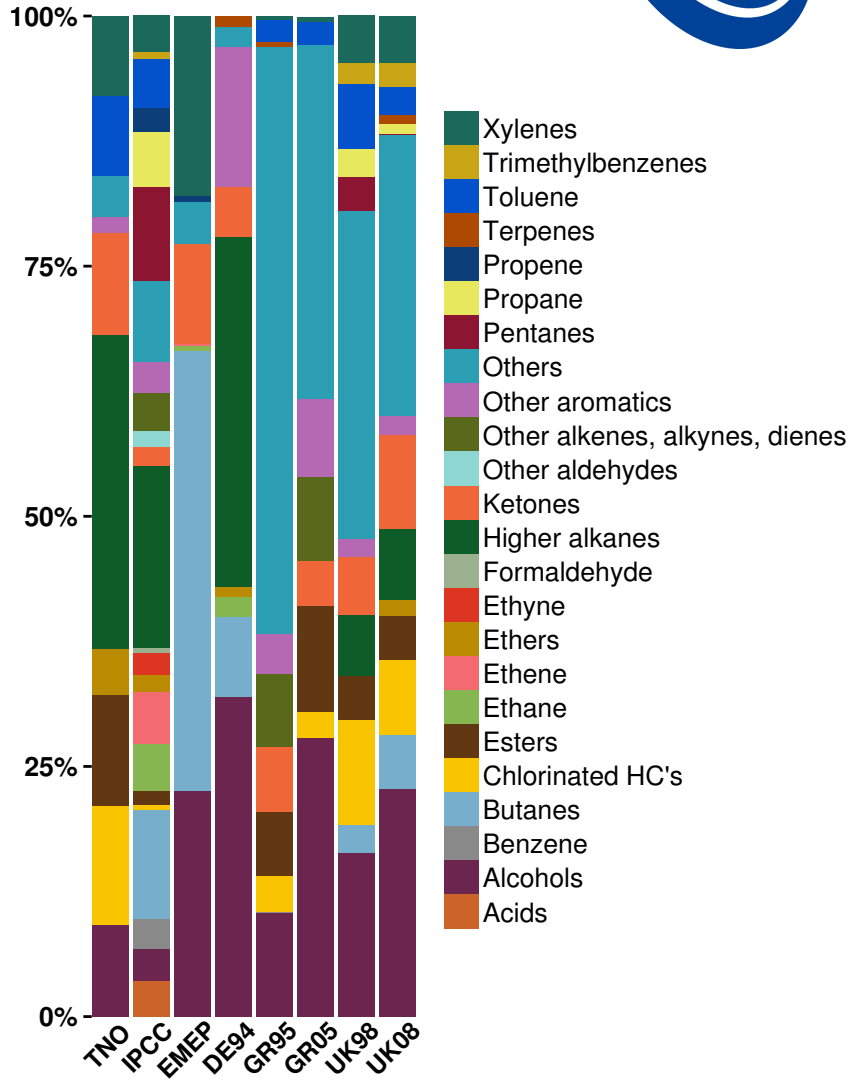
How does VOC speciation affect

O_3 concentrations in models?

Motivation



EEA Report, 2011



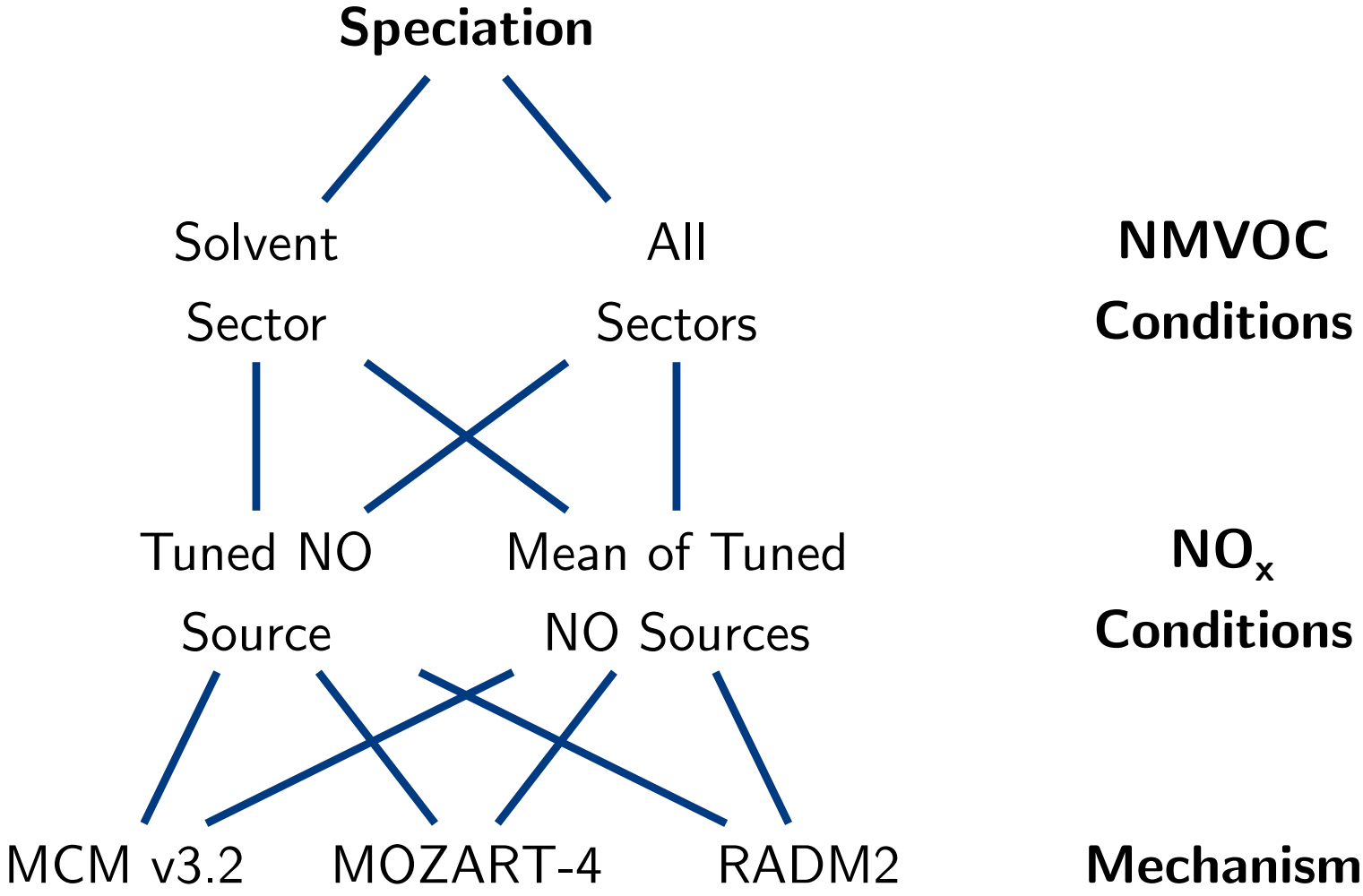
Compared Solvent Speciations

Speciation	Reference
TNO	[Builtjes et al., TNO Report, 2002]
IPCC	[Ehhalt et al., IPCC Report, 2001]
EMEP	[Simpson et al., ACP, 2010]
DE94	[Friedrich et. al., JAC, 2002]
GR95	[Sidiropoulos and Tsilingiridis, FEB, 2007]
GR05	[Sidiropoulos and Tsilingiridis, FEB, 2007]
UK98	[Goodwin, UK NAEI report, 2000]
UK08	[Murrells et al., UK NAEI Report, 2010]

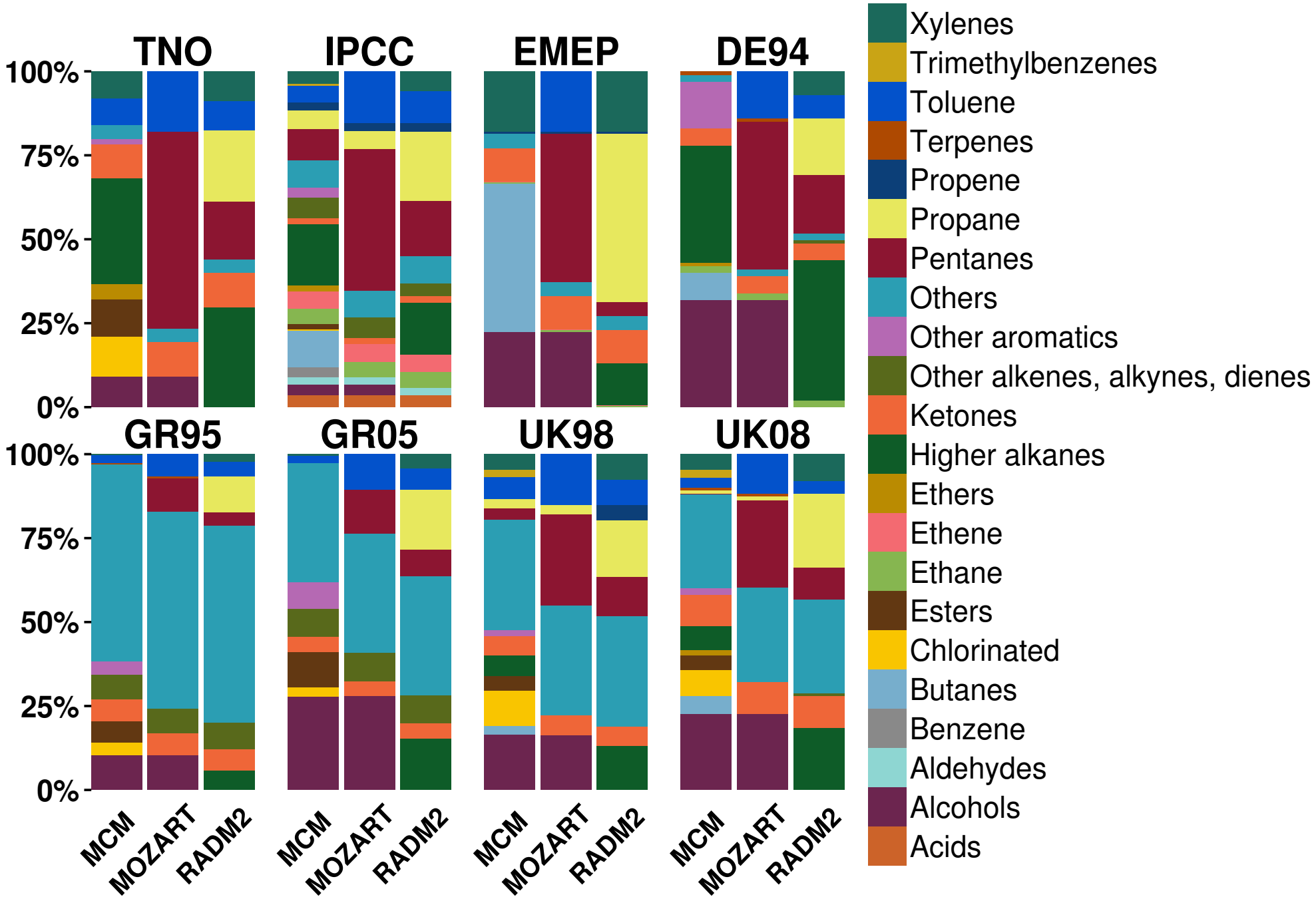
Boxmodel Setup

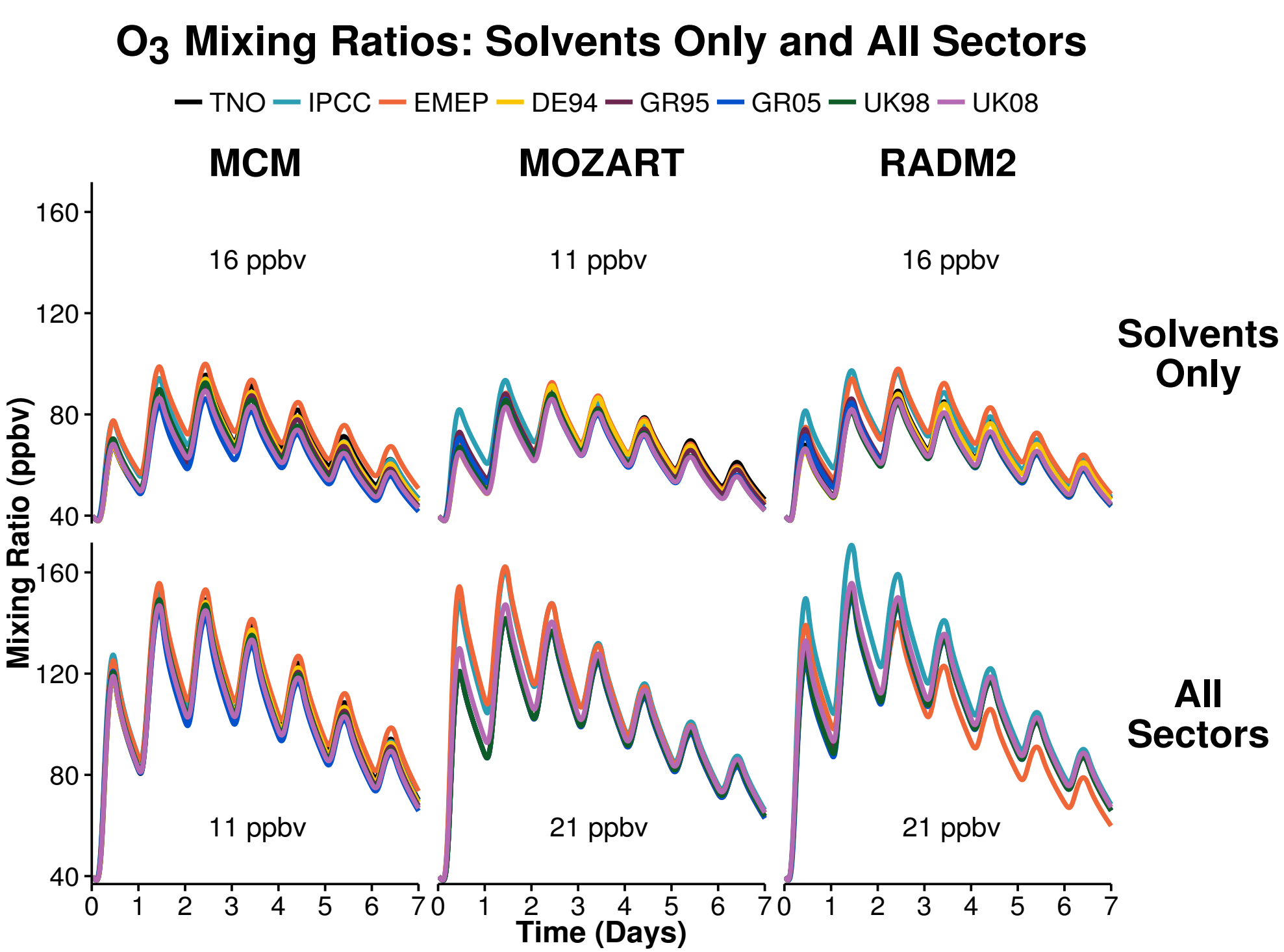
- MECCA boxmodel over 7 days.
- Idealised urban area of 1000 km^2.
- Total NMVOC emissions of 1000 ton/day [Warnecke et al., JGR, 2007].
- NMVOC emissions constant until noon of day 1.

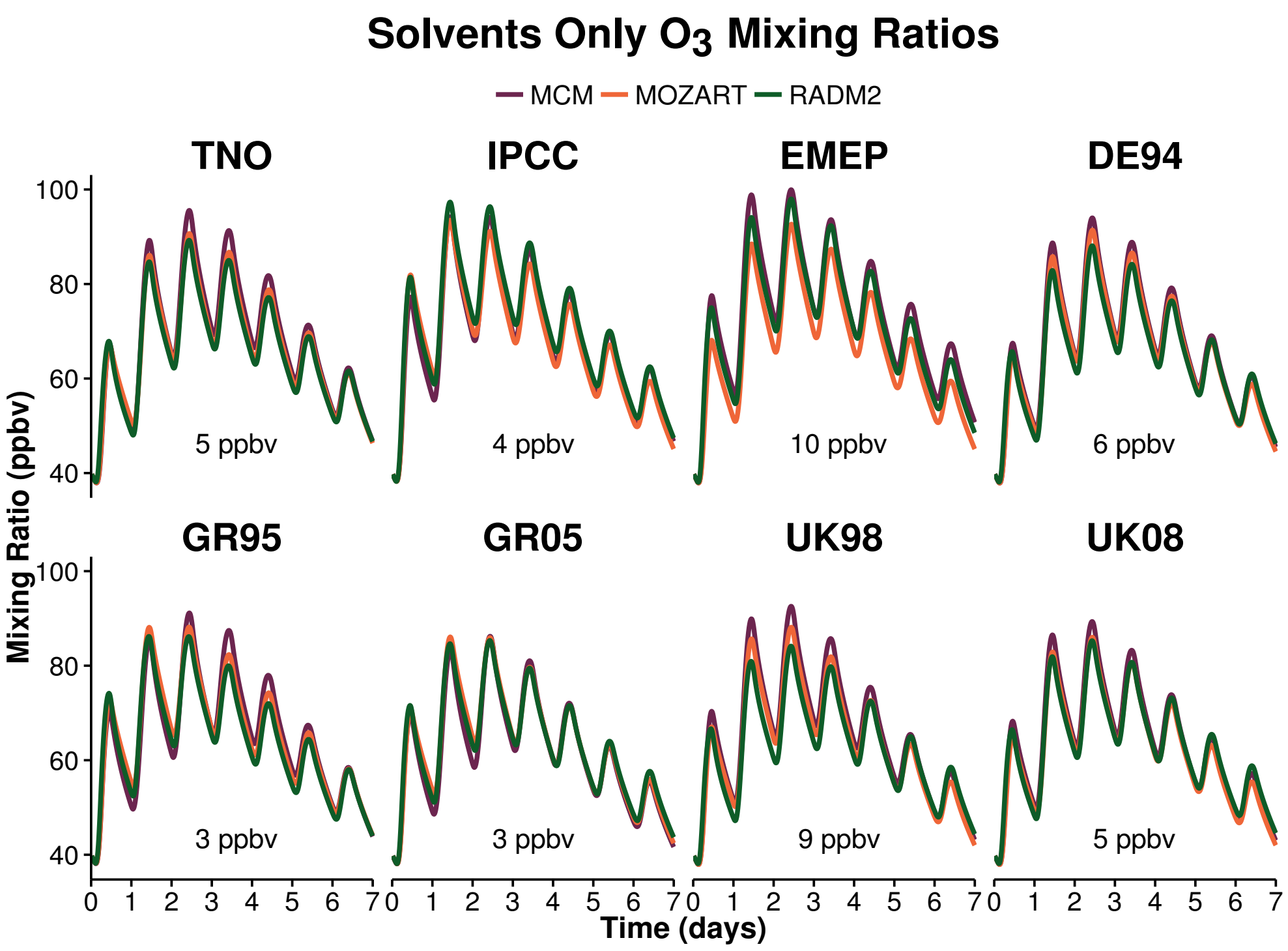
Model Scenarios



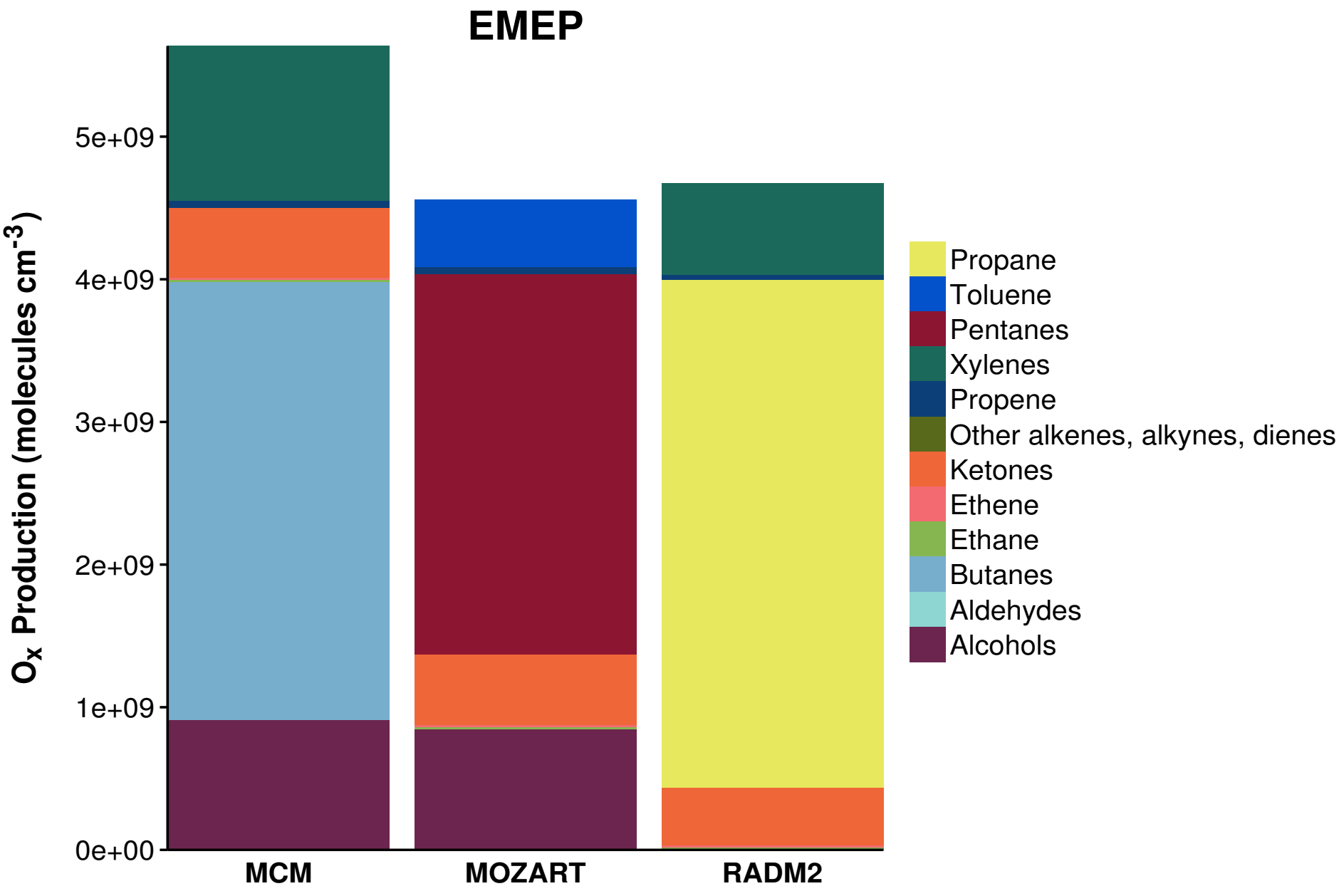
Solvent Speciations in Different Mechanisms



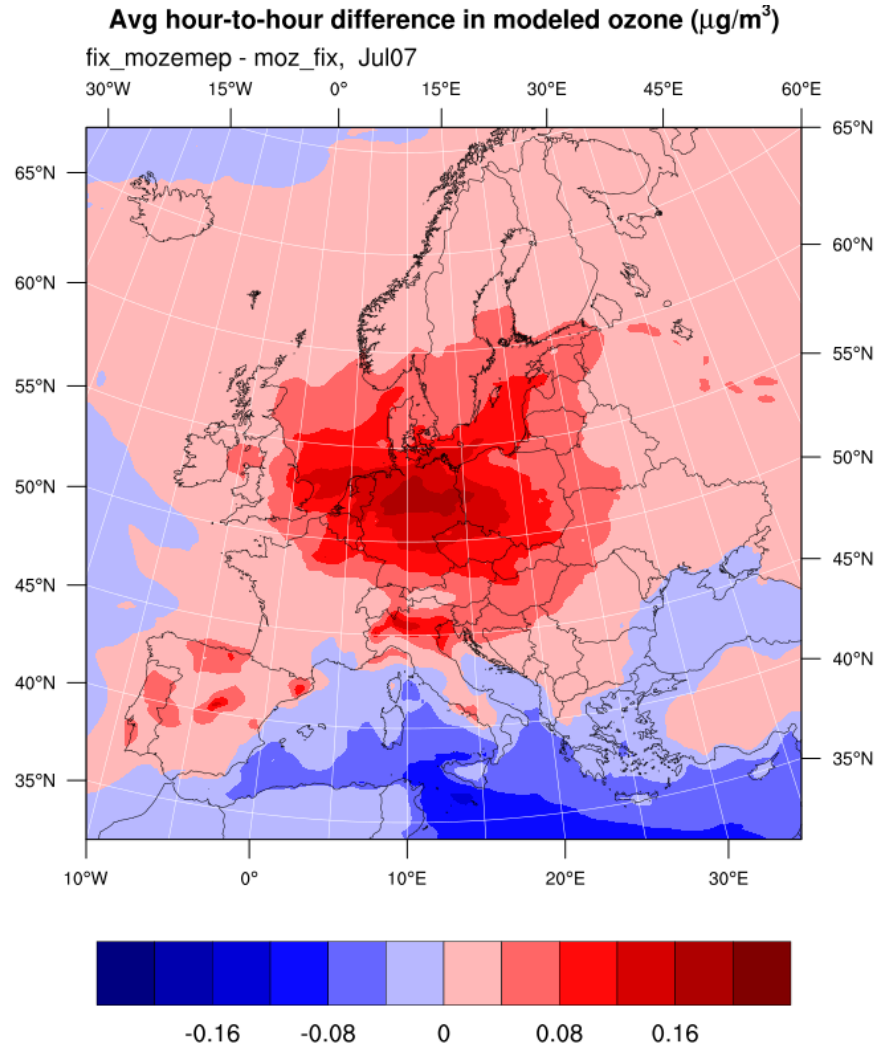

O3 Mixing Ratios: Solvents Only and All Sectors
TNO
IPCC
EMEP
DE94
GR95
GR05
UK98
UK08
MCM
MOZART
RADM2
Solvents Only
All Sectors
Mixing Ratio (ppbv)
Time (Days)
16 ppbv
11 ppbv
16 ppbv
11 ppbv
21 ppbv
21 ppbv
160
120
80
40
0
1
2
3
4
5
6
7


Solvents Only O_3 Mixing Ratios
MCM
MOZART
RADM2
TNO
IPCC
EMEP
DE94
GR95
GR05
UK98
UK08
5 ppbv
4 ppbv
10 ppbv
6 ppbv
3 ppbv
3 ppbv
9 ppbv
5 ppbv
Mixing Ratio (ppbv)
Time (days)
100
80
60
40
0
1
2
3
4
5
6
7

Solvents Only: Cumulative O_X Production Budget



Further Analysis



- Representation of VOC between mechanisms, e.g. chlorinated VOC.
- Reasons for large differences in boxmodel results, given the regional modelling results.

Outline

Other Contributions

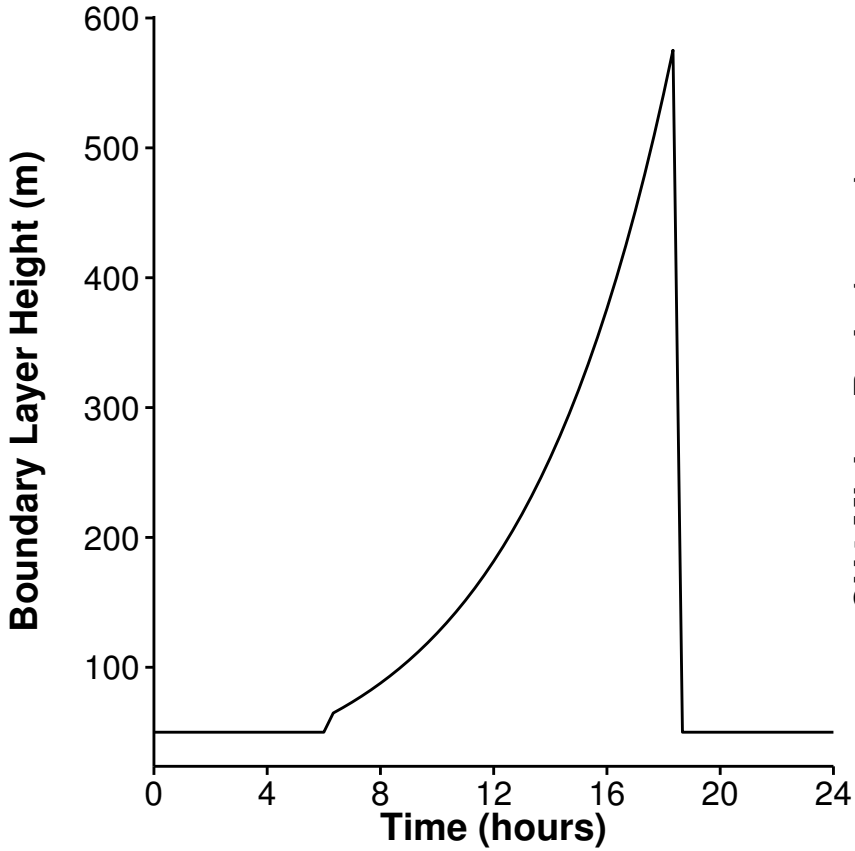
- Presentations and Posters
  - Poster and presentation at PhD Conference on Earth System Science, Mar 2014.
  - Poster at IASS Evaluation, May 2014.
  - Poster at Our Climate Our Future (REKLIM) Conference, Oct 2014.
  - Presentation at OH Reactivity Specialists Uniting Meeting (ORSUM), Oct 2014.
- 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.

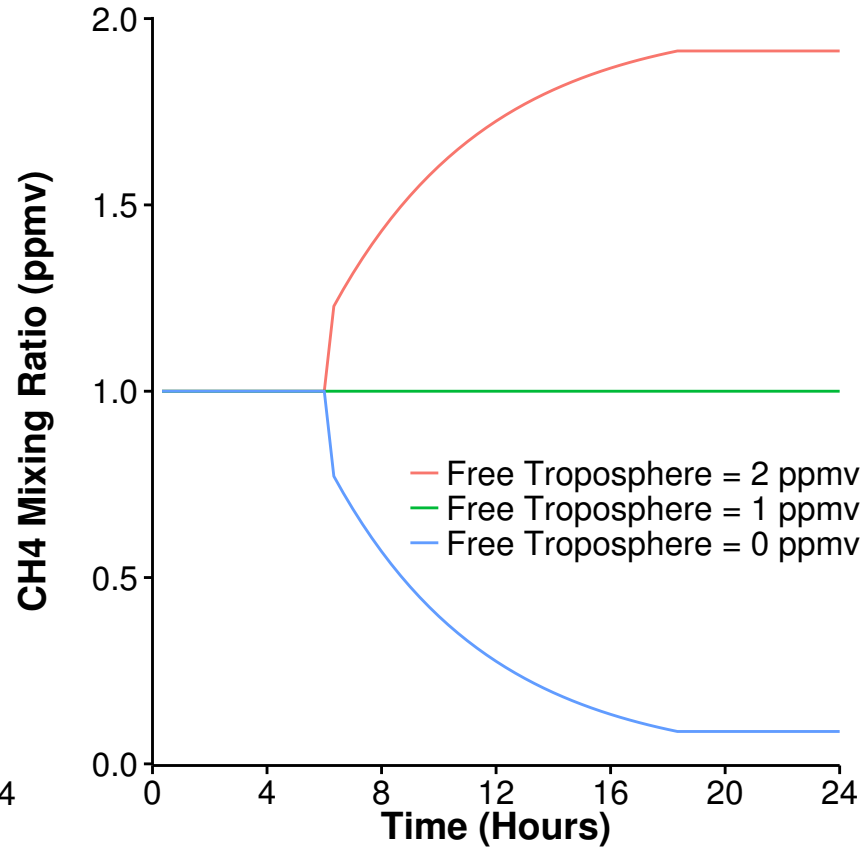
Outline

Future Modelling

- Realistic Conditions
  - Include diurnal cycle of boundary layer height and vertical mixing.
  - CARES data for NO_x and VOC conditions?
- Variable meteorological parameters (temperature, solar radiation).
- O_x production in different atmospheric regimes.
- Tagging approach used in global model.

Future Modelling: Vertical Mixing

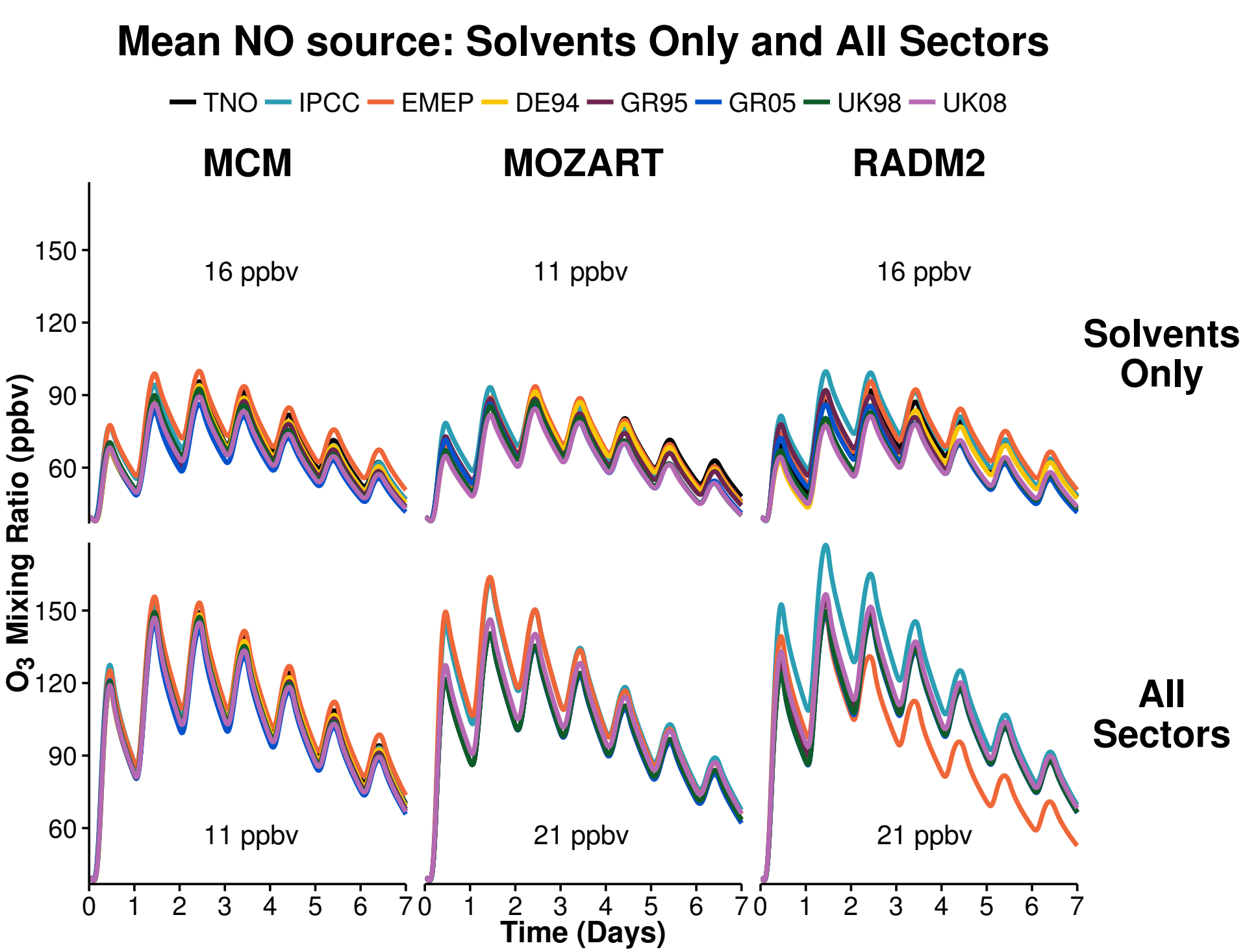


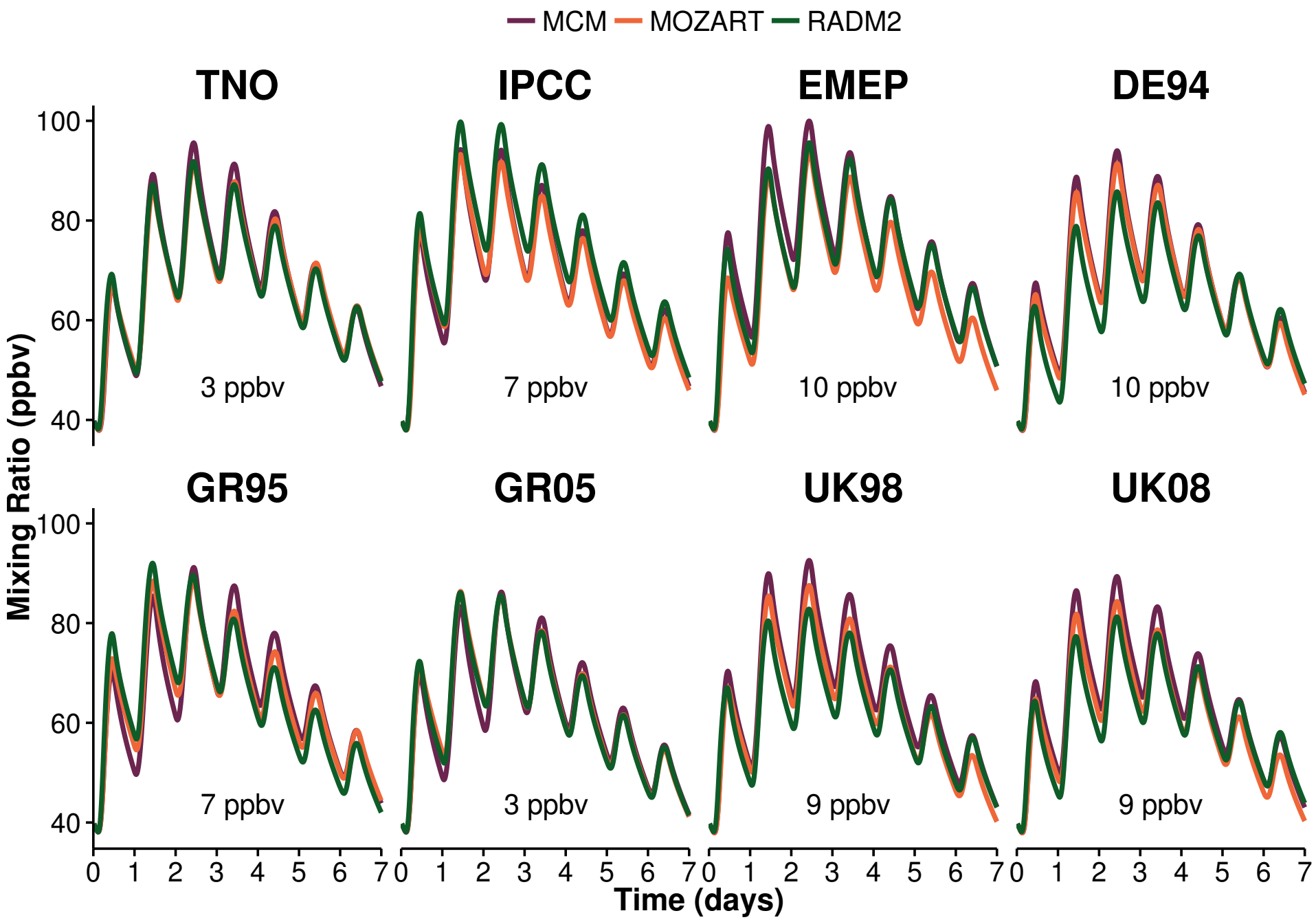


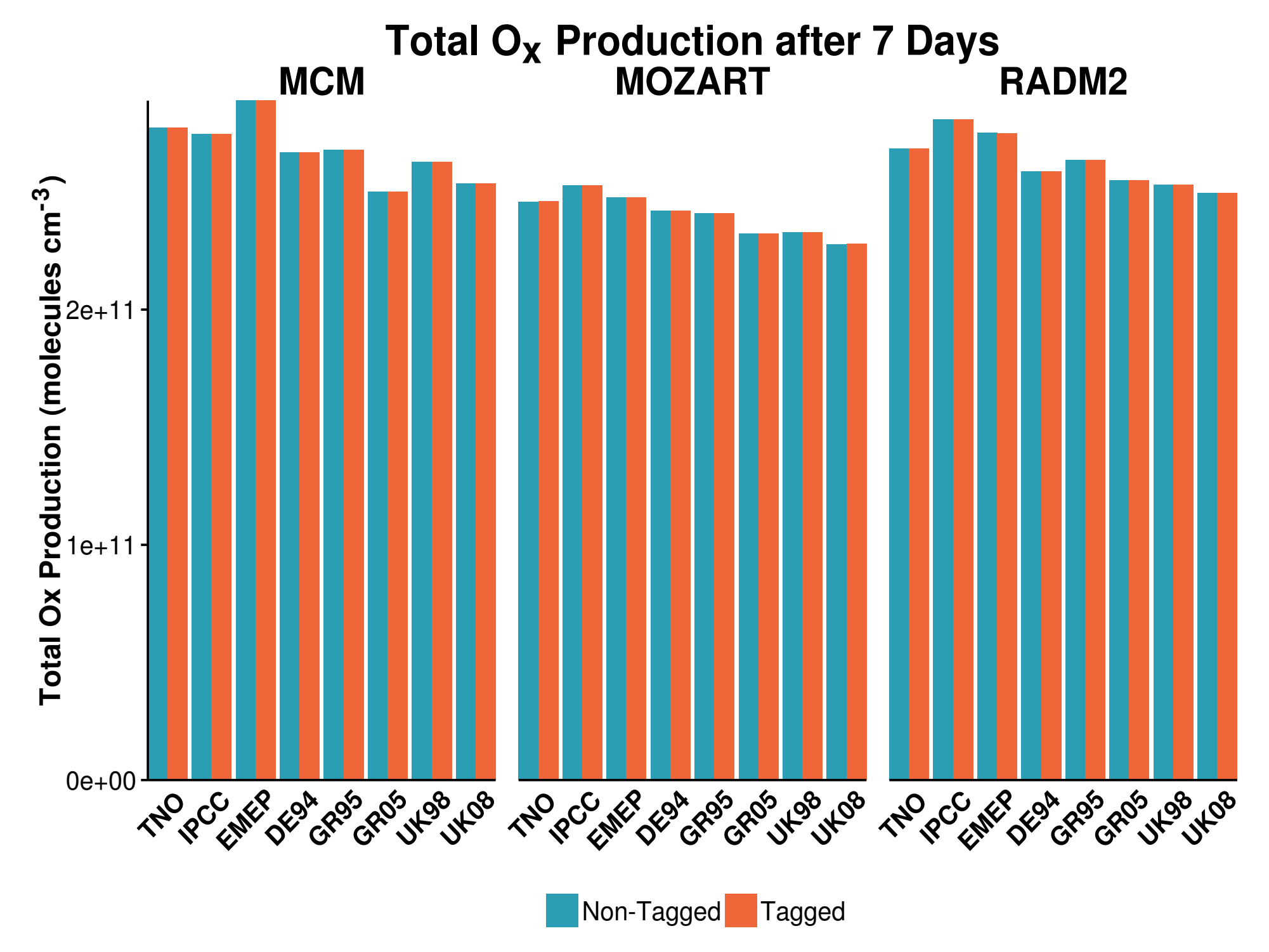
Future Writing

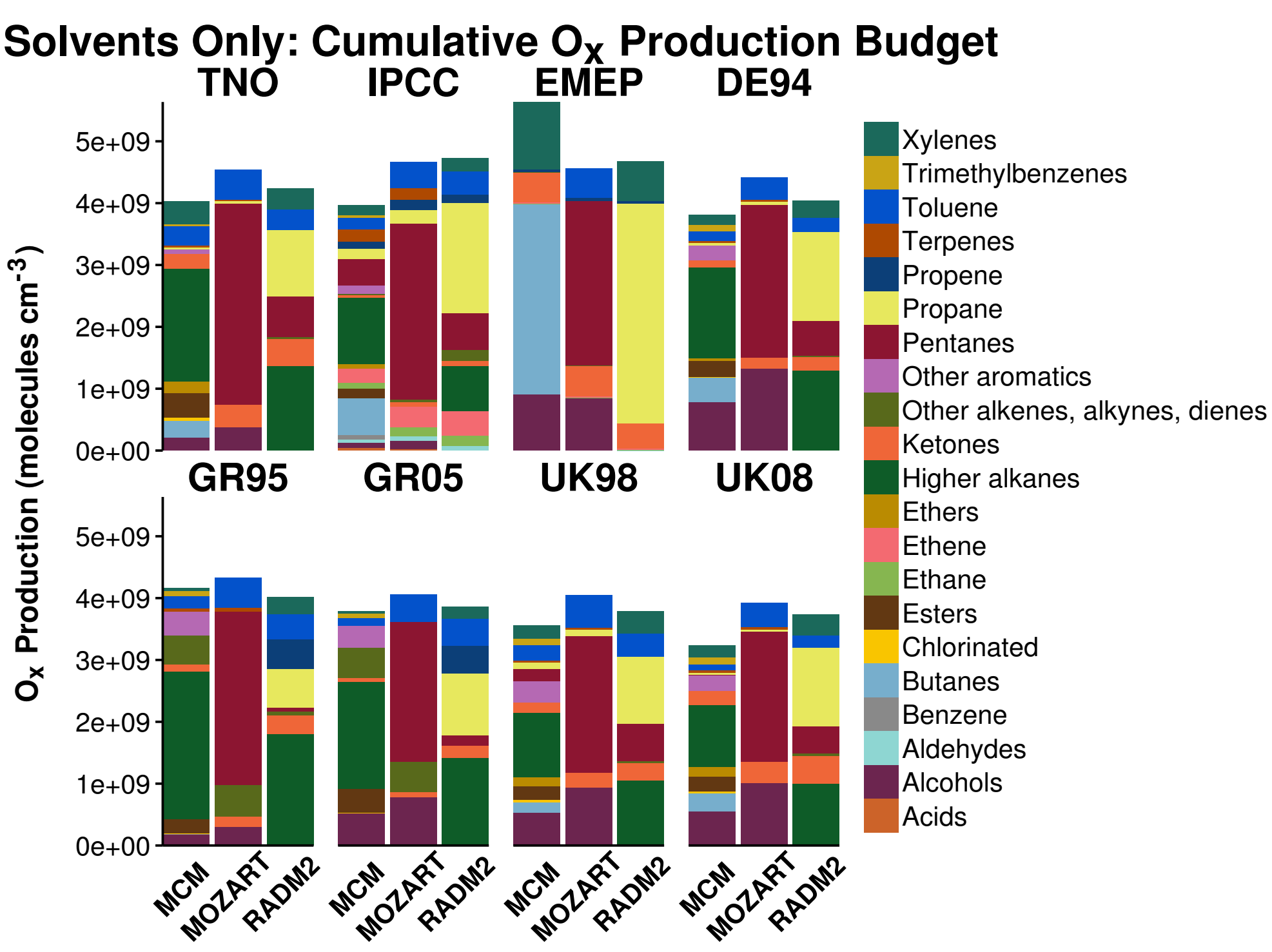
- Attending 'Scientific Writing for Advanced Doctoral Students' course organised by Galina Churkina.
- Solvent speciations paper with Erika von Schneidemesser.
- Final paper.
- Thesis.

Extra Slides


Mean NO source: Solvents Only and All Sectors
TNO
IPCC
EMEP
DE94
GR95
GR05
UK98
UK08
MCM
MOZART
RADM2
Solvents Only
All Sectors
16 ppbv
11 ppbv
16 ppbv
11 ppbv
21 ppbv
21 ppbv
O3 Mixing Ratio (ppbv)
Time (Days)
150
120
90
60
0
1
2
3
4
5
6
7


Mean NO Source: Solvents Only O_3 Mixing Ratios
MCM
MOZART
RADM2
TNO
IPCC
EMEP
DE94
GR95
GR05
UK98
UK08
3 ppbv
7 ppbv
10 ppbv
10 ppbv
7 ppbv
3 ppbv
9 ppbv
9 ppbv
Mixing Ratio (ppbv)
Time (days)
40
60
80
100
0
1
2
3
4
5
6
7


Total O_x Production after 7 Days
MCM
MOZART
RADM2
Total Ox Production (molecules cm^{-3})
0e+00
1e+11
2e+11
TNO
IPCC
EMEP
DE94
GR95
GR05
UK98
UK08
Non-Tagged
Tagged


Solvents Only: Cumulative O_X Production Budget
TNO
IPCC
EMEP
DE94
GR95
GR05
UK98
UK08
O_X Production (molecules cm^{-3})
0e+00
1e+09
2e+09
3e+09
4e+09
5e+09
MCM
MOZART
RADM2
Xylenes
Trimethylbenzenes
Toluene
Terpenes
Propene
Propane
Pentanes
Other aromatics
Other alkenes, alkynes, dienes
Ketones
Higher alkanes
Ethers
Ethene
Ethane
Esters
Chlorinated
Butanes
Benzene
Aldehydes
Alcohols
Acids

Thesis

- Created base structure based on Andrea's thesis.
- Started introduction using literature review.
- Planning structure using mind map.