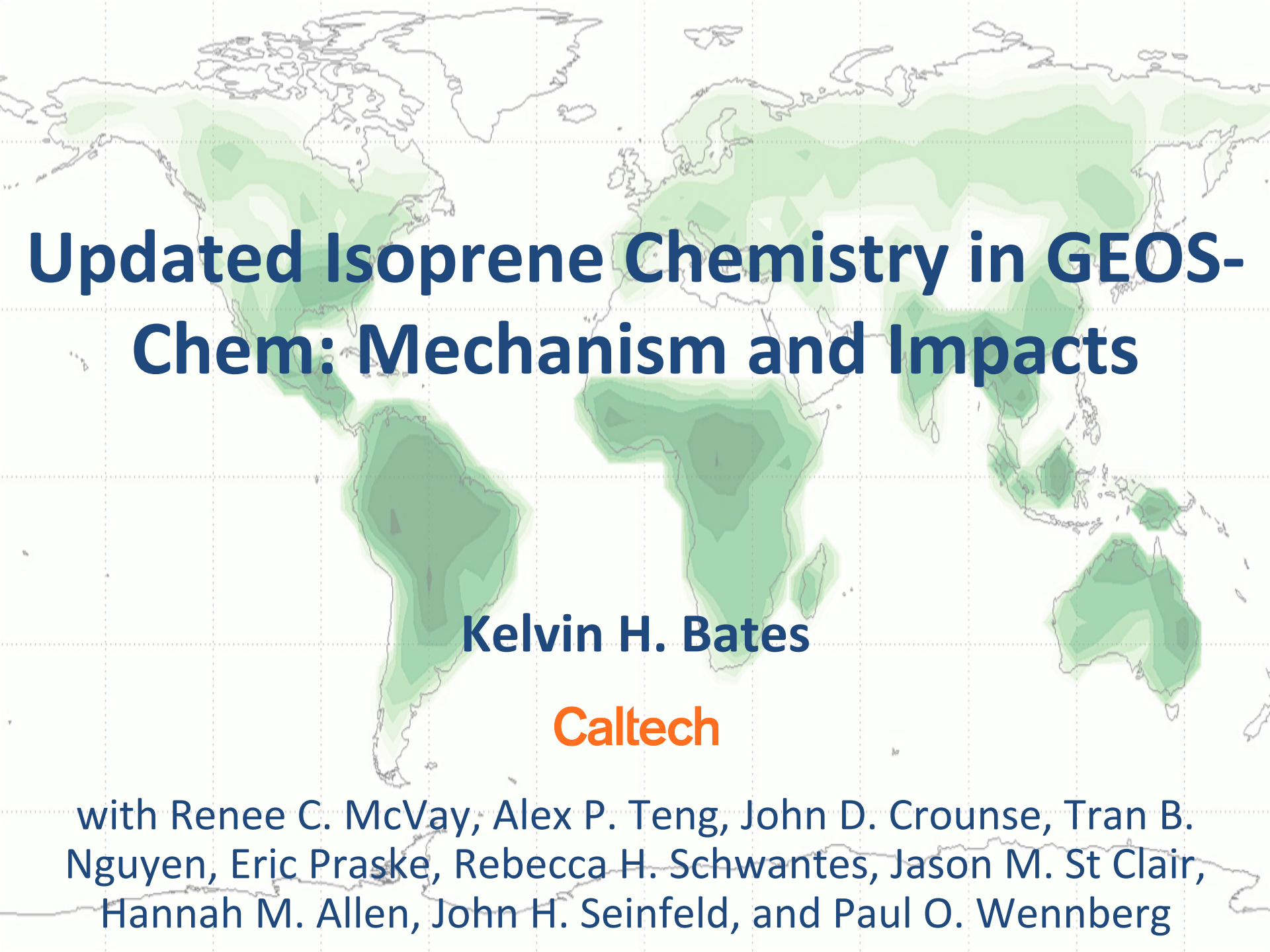


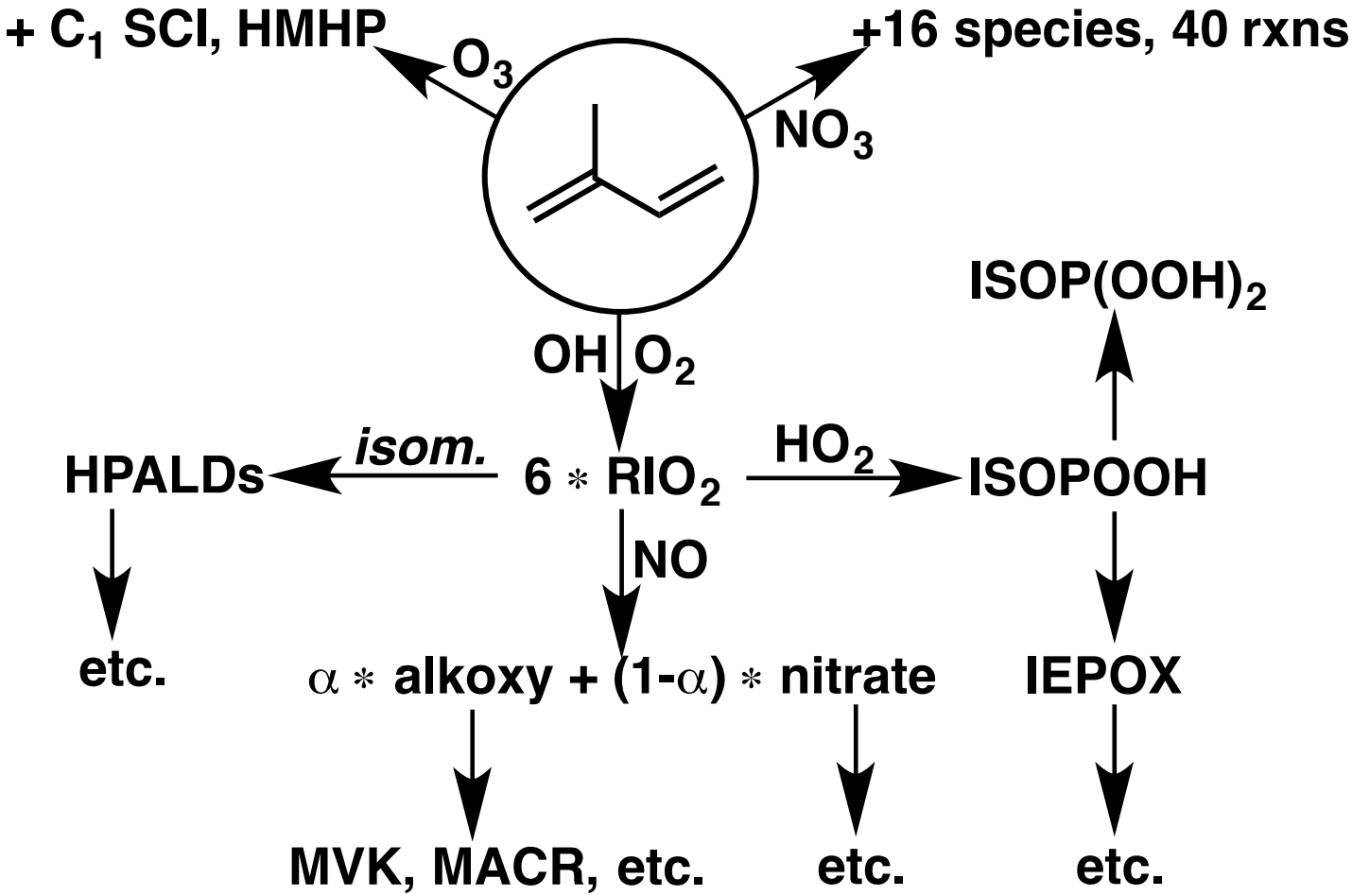
Updated Isoprene Chemistry in GEOS-Chem: Mechanism and Impacts

Kelvin H. Bates

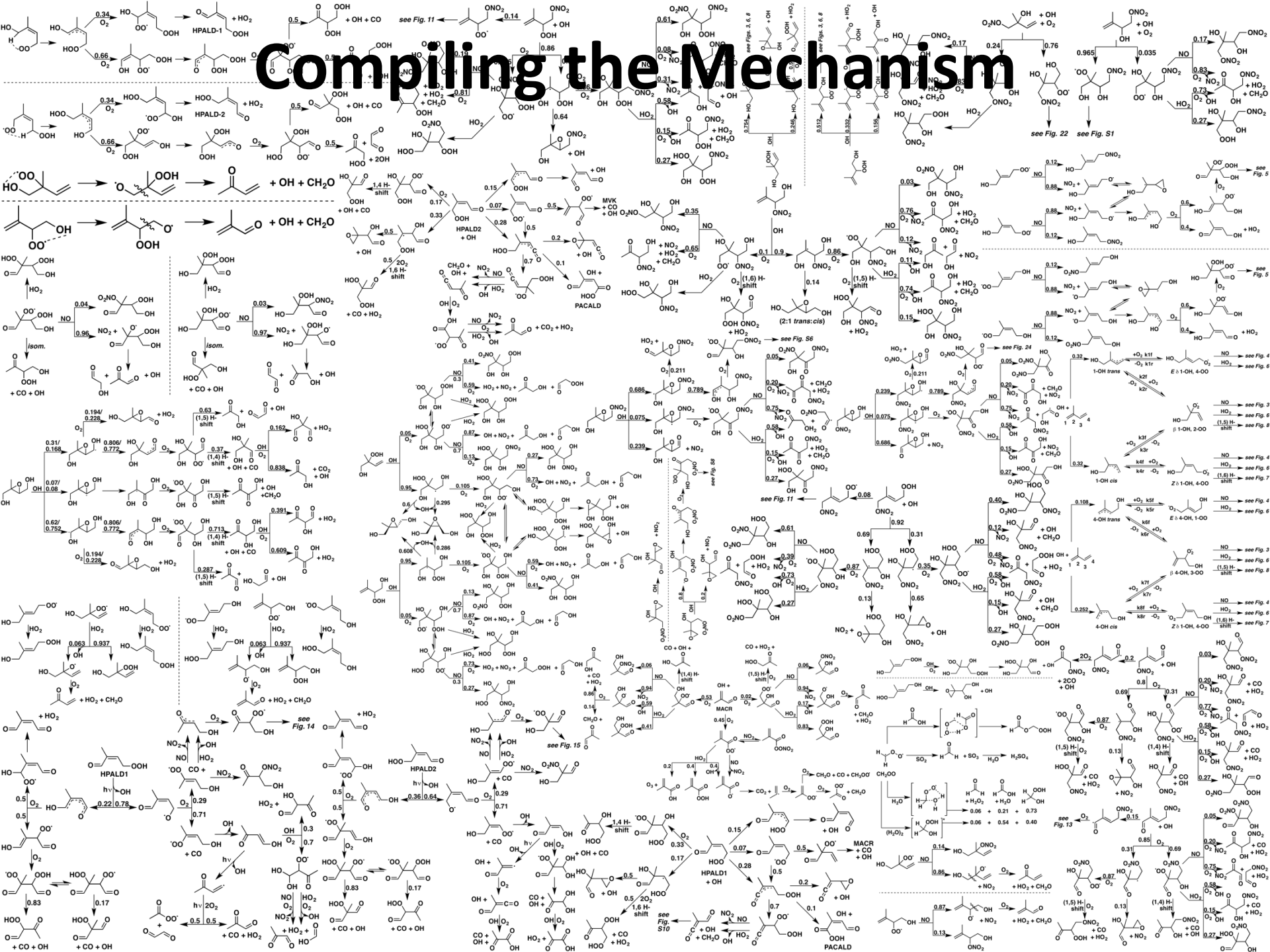
Caltech

with Renee C. McVay, Alex P. Teng, John D. Crounse, Tran B. Nguyen, Eric Praske, Rebecca H. Schwantes, Jason M. St Clair, Hannah M. Allen, John H. Seinfeld, and Paul O. Wennberg

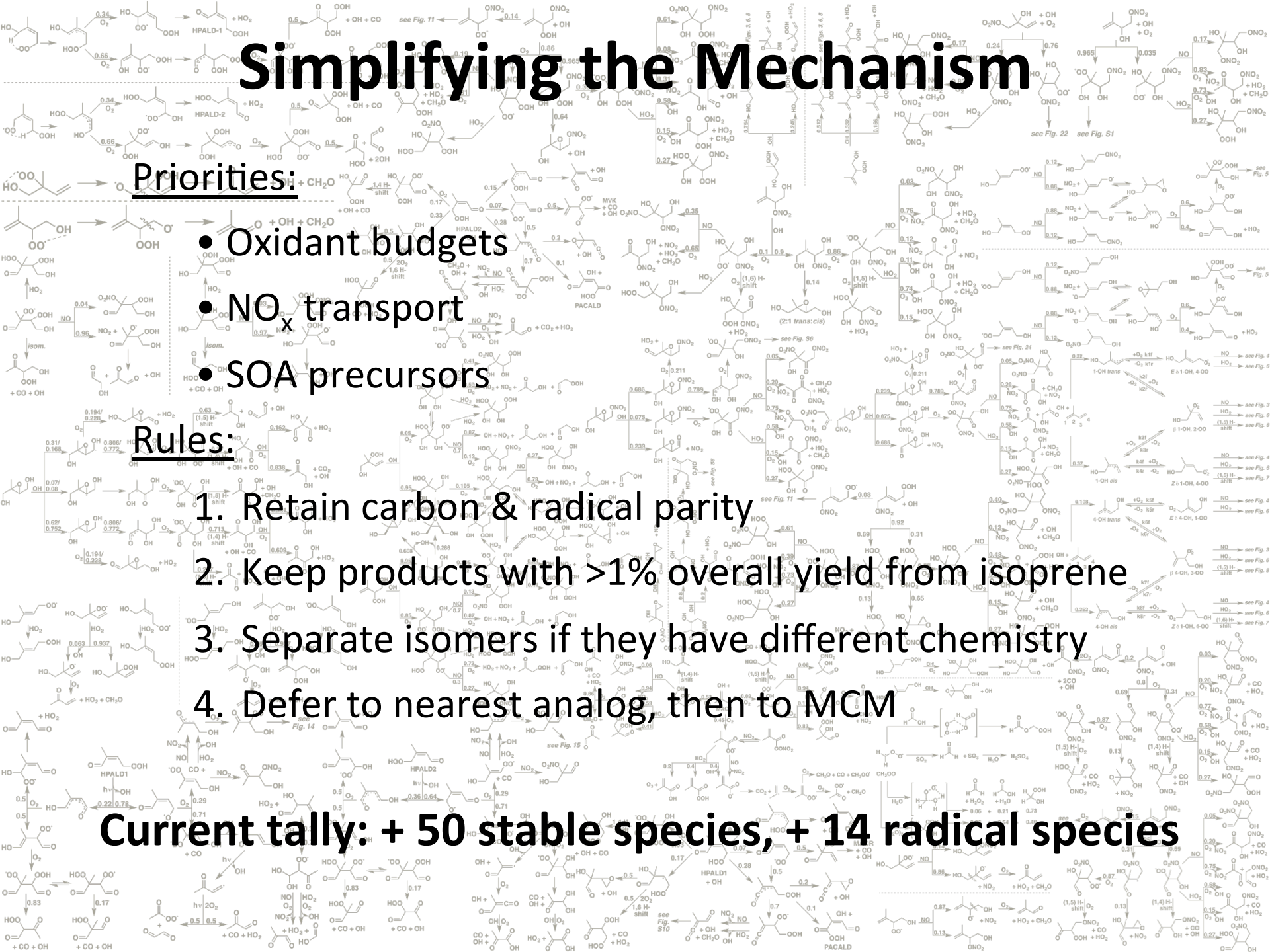
Compiling the Mechanism



J. St. Clair *et al.*, J. Phys. Chem. A, 2015; A. Teng *et al.*, J. Am. Chem. Soc. , 2017;
T. Nguyen *et al.*, Phys. Chem. Chem. Phys., 2015; K. Bates *et al.*, J Phys. Chem. A, 2016; K. Bates *et al.*, J Phys. Chem. A, 2014
A. Teng *et al.*, Atmos. Chem. Phys., 2015; L. Lee *et al.*, J. Phys. Chem. A, 2014; E. Praske *et al.*, J. Phys. Chem. A, 2015
T. Nguyen *et al.*, PNAS, 2014; J. Peeters *et al.*, J. Phys. Chem. A, 2014; J. Crounse *et al.*, Phys. Chem. Chem. Phys., 2011
T. Nguyen *et al.*, Phys. Chem. Chem. Phys., 2016; H. Allen *et al.*, in prep, 2017; R. Schwantes *et al.*, J. Phys. Chem. A, 2016


Compiling the Mechanism

Simplifying the Mechanism



Priorities:

- Oxidant budgets
- NO_x transport
- SOA precursors

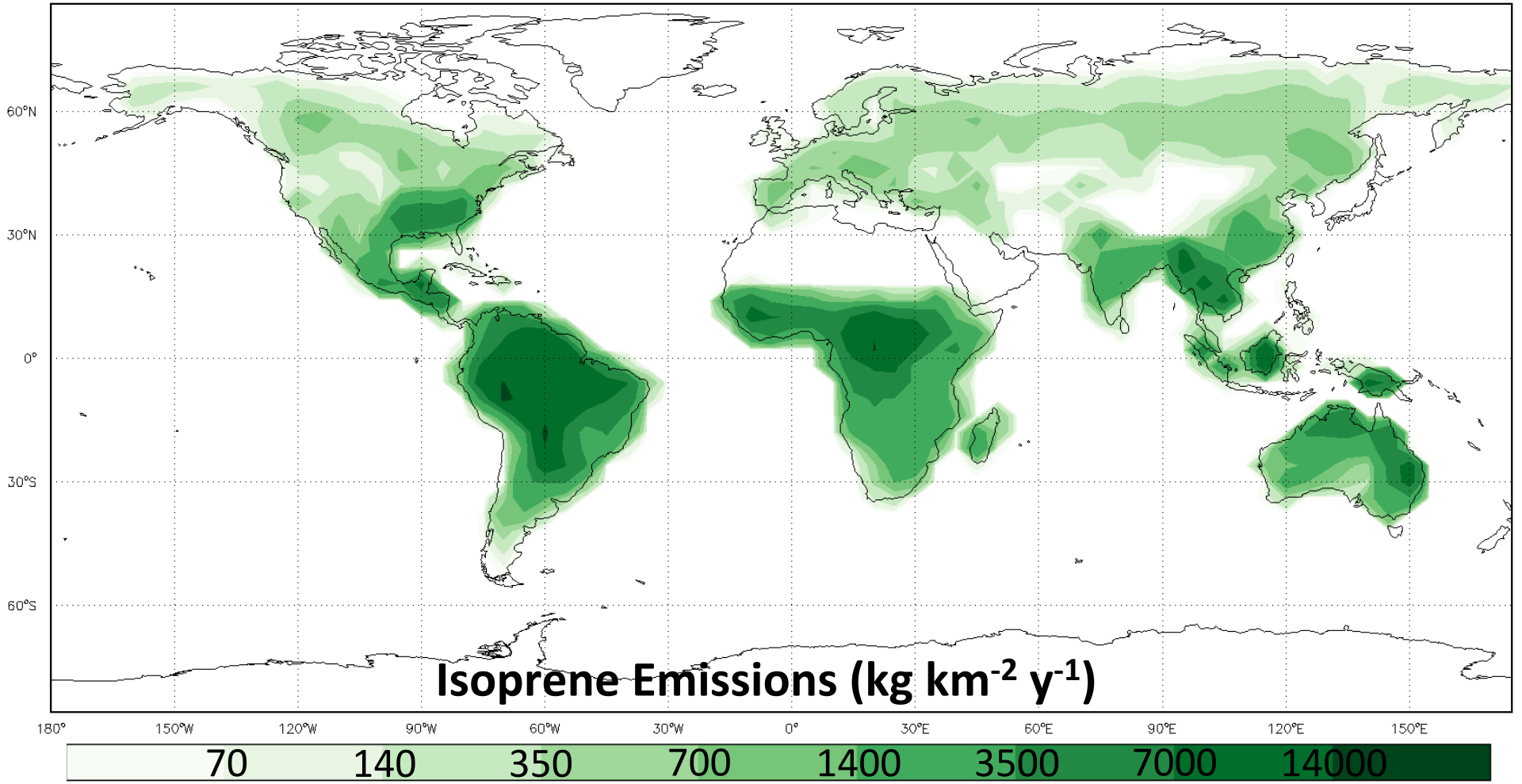
Rules:

1. Retain carbon & radical parity
2. Keep products with >1% overall yield from isoprene
3. Separate isomers if they have different chemistry
4. Defer to nearest analog, then to MCM

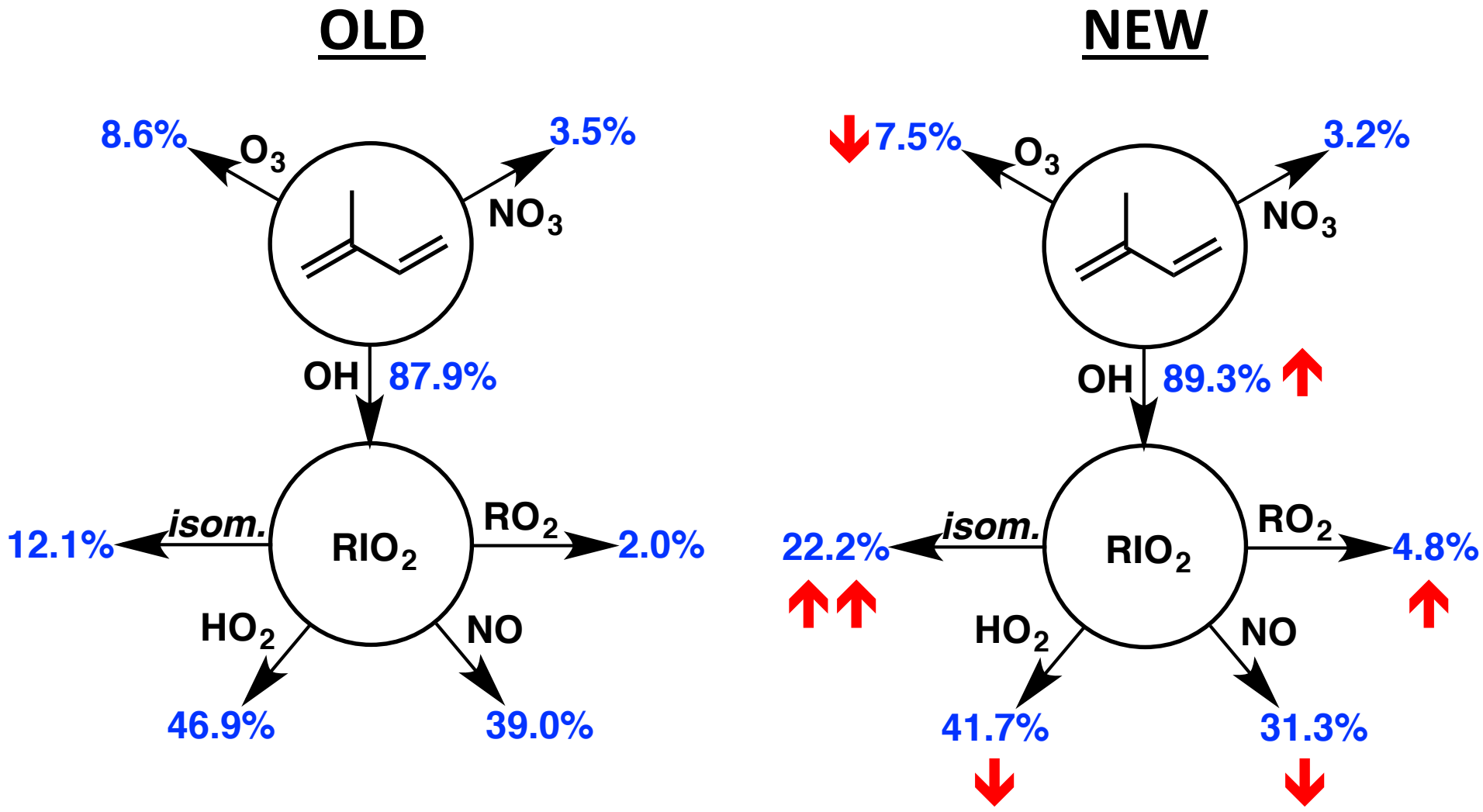
Current tally: + 50 stable species, + 14 radical species

Preliminary Results

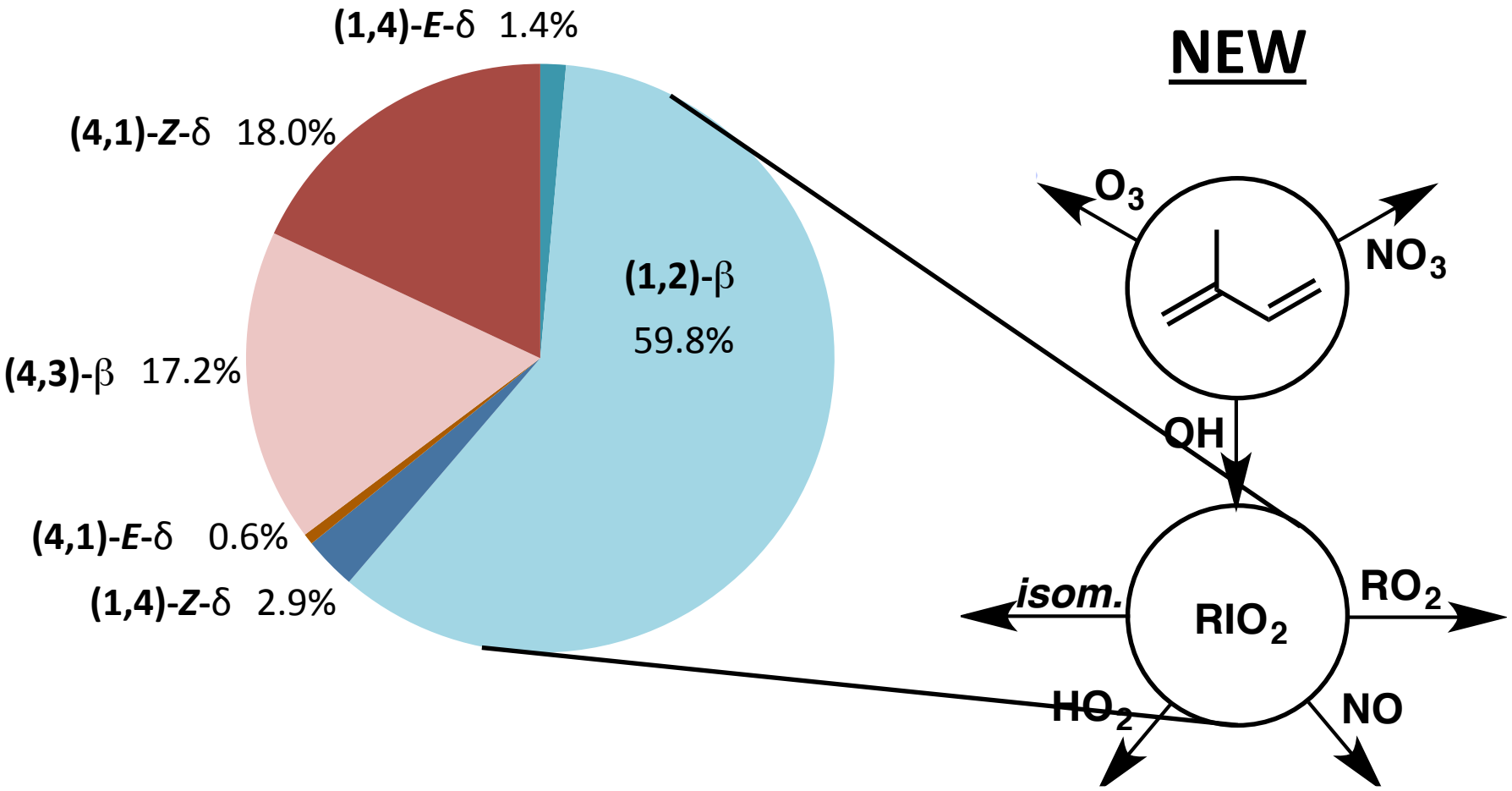
- v. 10-01
- 4˚x5˚ grid
- GEOS-FP meteorology
- annual average over 2014
- 1.5-year spinup



Preliminary Results: VOCs



Preliminary Results: VOCs



Preliminary Results: MVK/MACR

MVK

Production: ↑ 42.5%

Atmospheric loading:

Surface: ↑ 43.3%

Total: ↑ 47.4%

Methacrolein

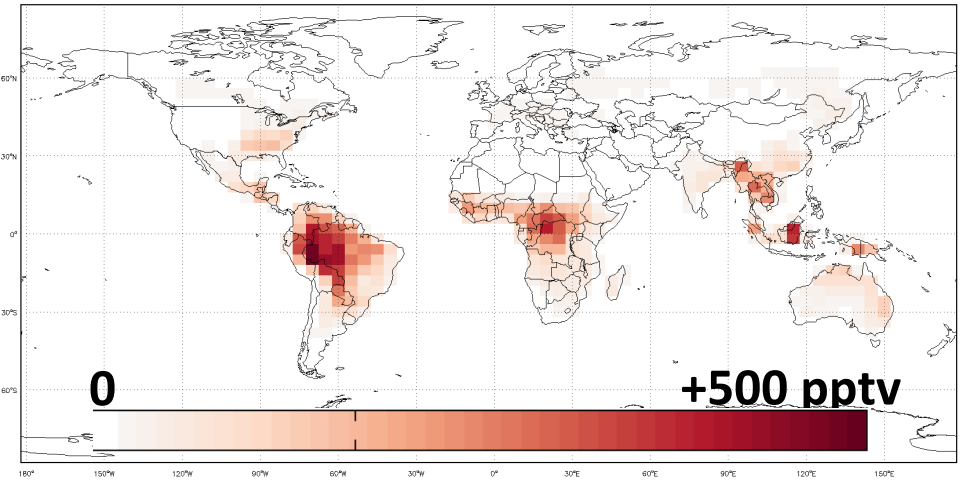
Production: ↓ 23.0%

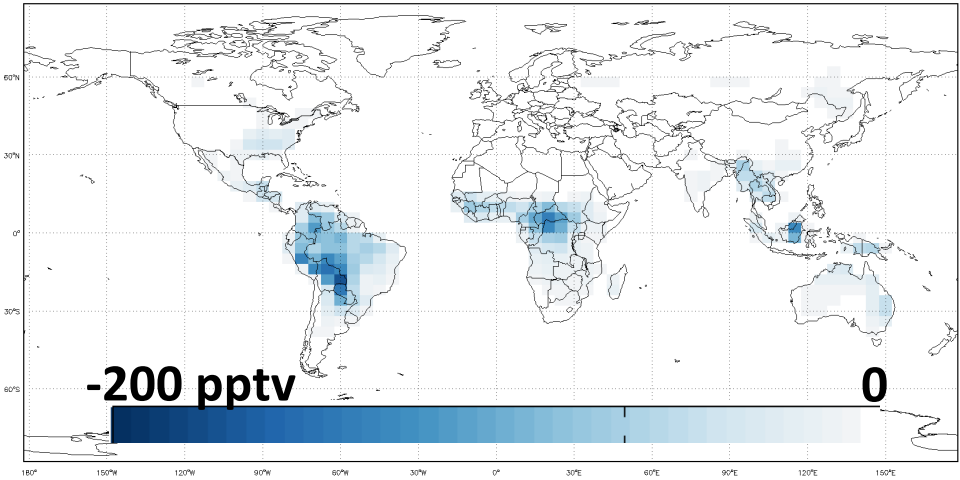
Atmospheric loading:

Surface: ↓ 25.7%

Total: ↓ 23.5%

Absolute change at surface from old to new isoprene mechanism, 2014

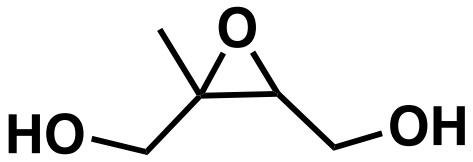




[MVK]/[MACR] ratio nearly doubles from 1.38 to 2.57

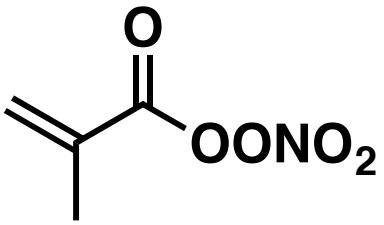
Preliminary Results: SOA Precursors

IEPOX



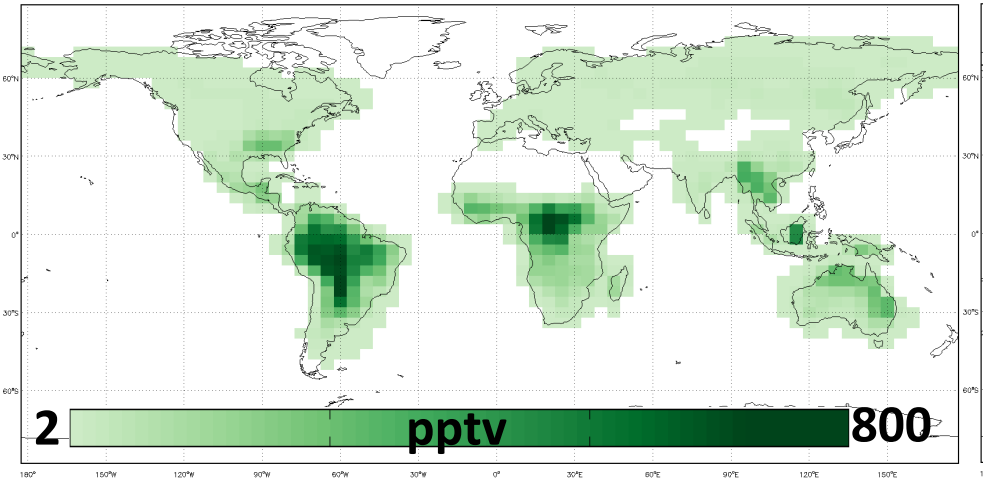
Production: 183 Tg y^{-1} (↓ 19%)

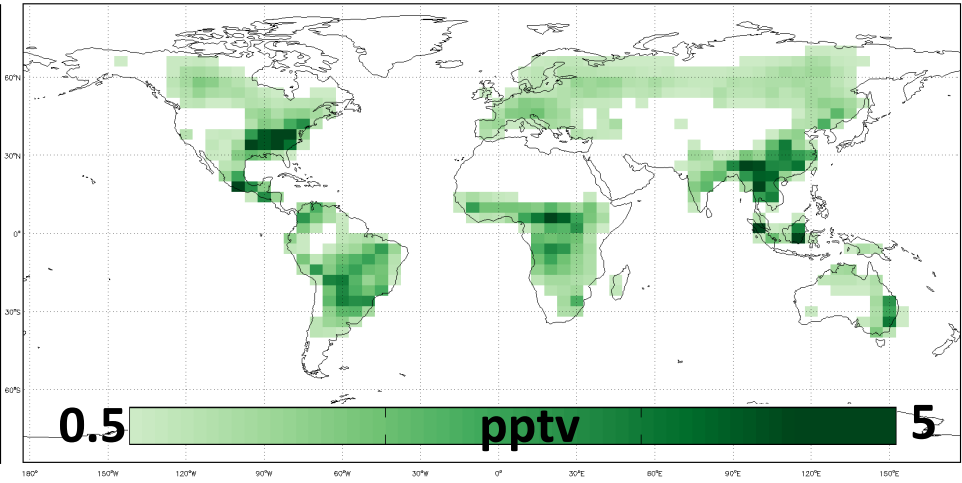
MPAN



Production: 32.7 Tg y^{-1} (↑ 29%)

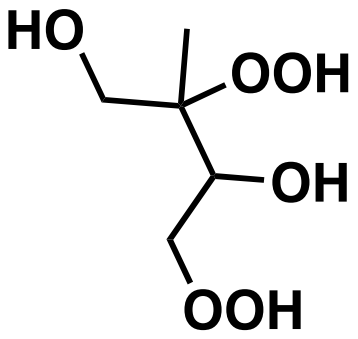
Annual average pptv in lowest 1 km, 2014

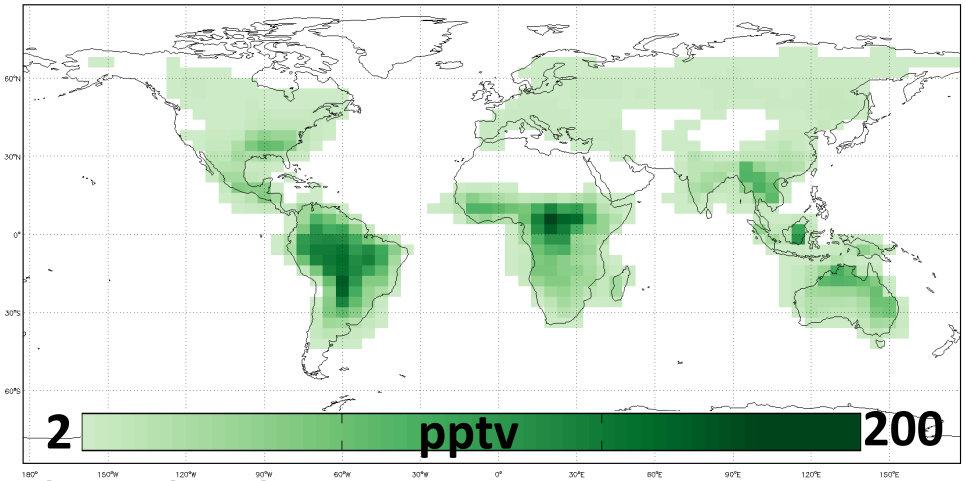


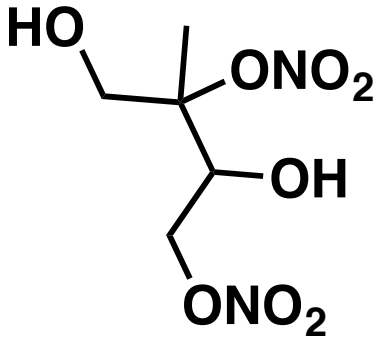


Preliminary Results: SOA Precursors

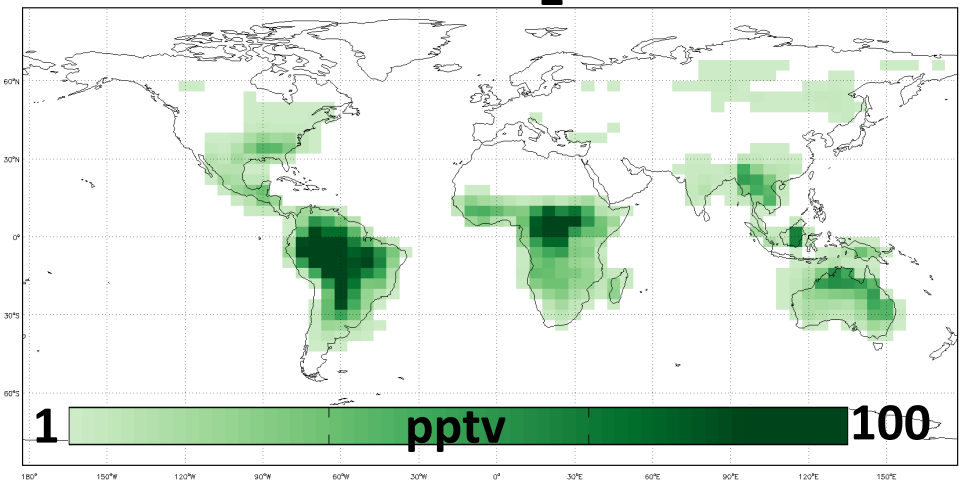
Tetrafunctionals: 44.2 Tg y^{-1}



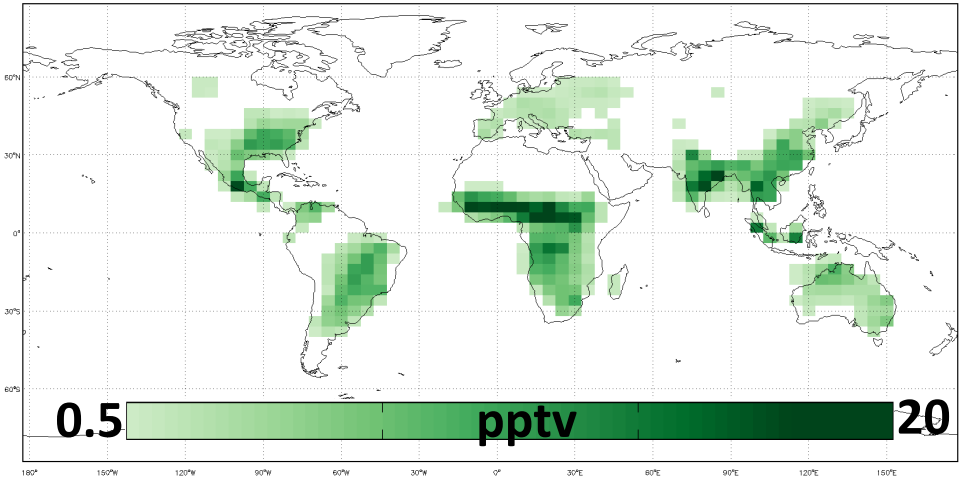




$ISOP(OOH)_2$ (*2)



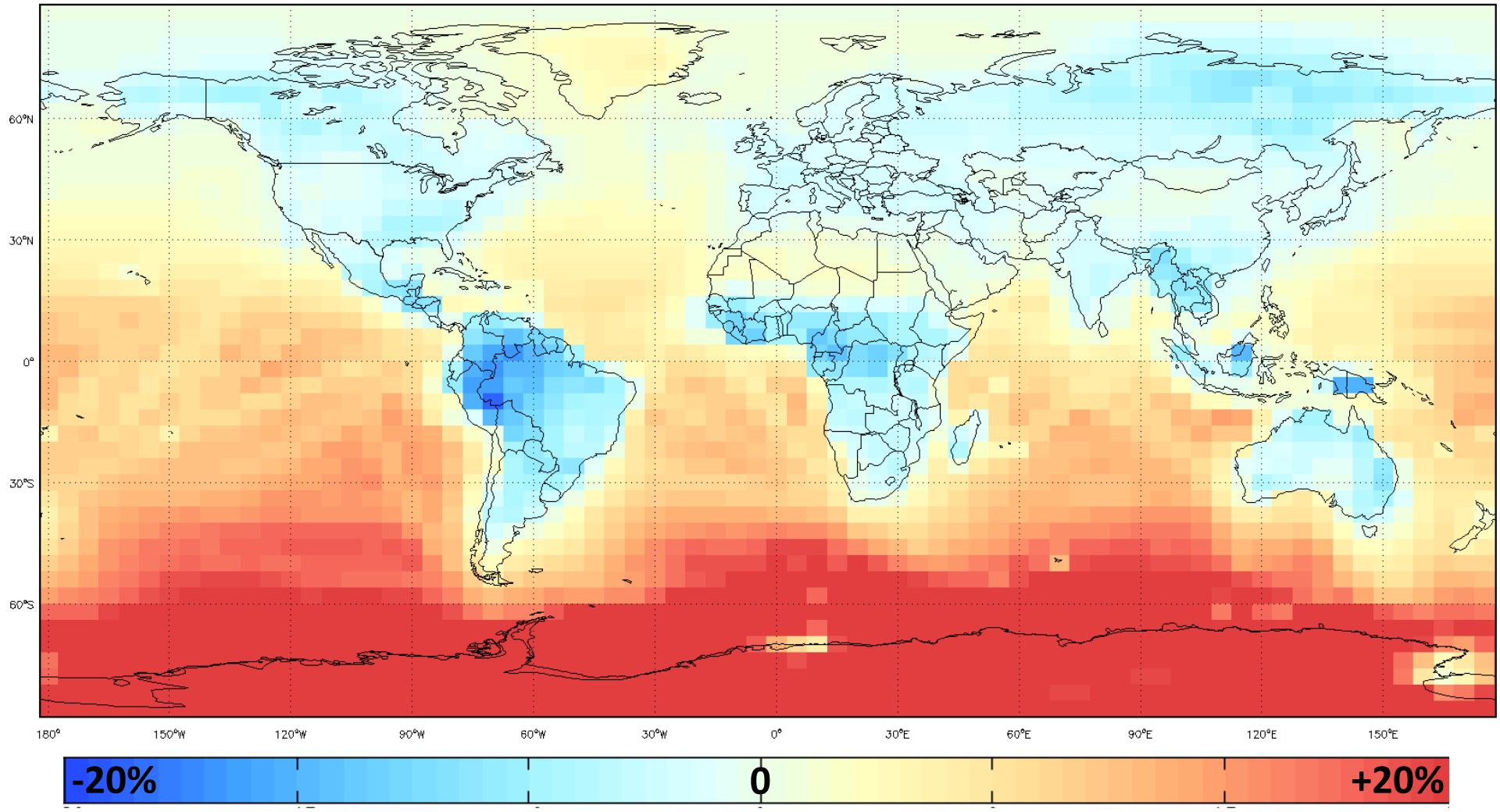
Dihydroxy-dinitrates (*10)



Annual average pptv in lowest 1 km, 2014

Preliminary Results: Δ NO_x

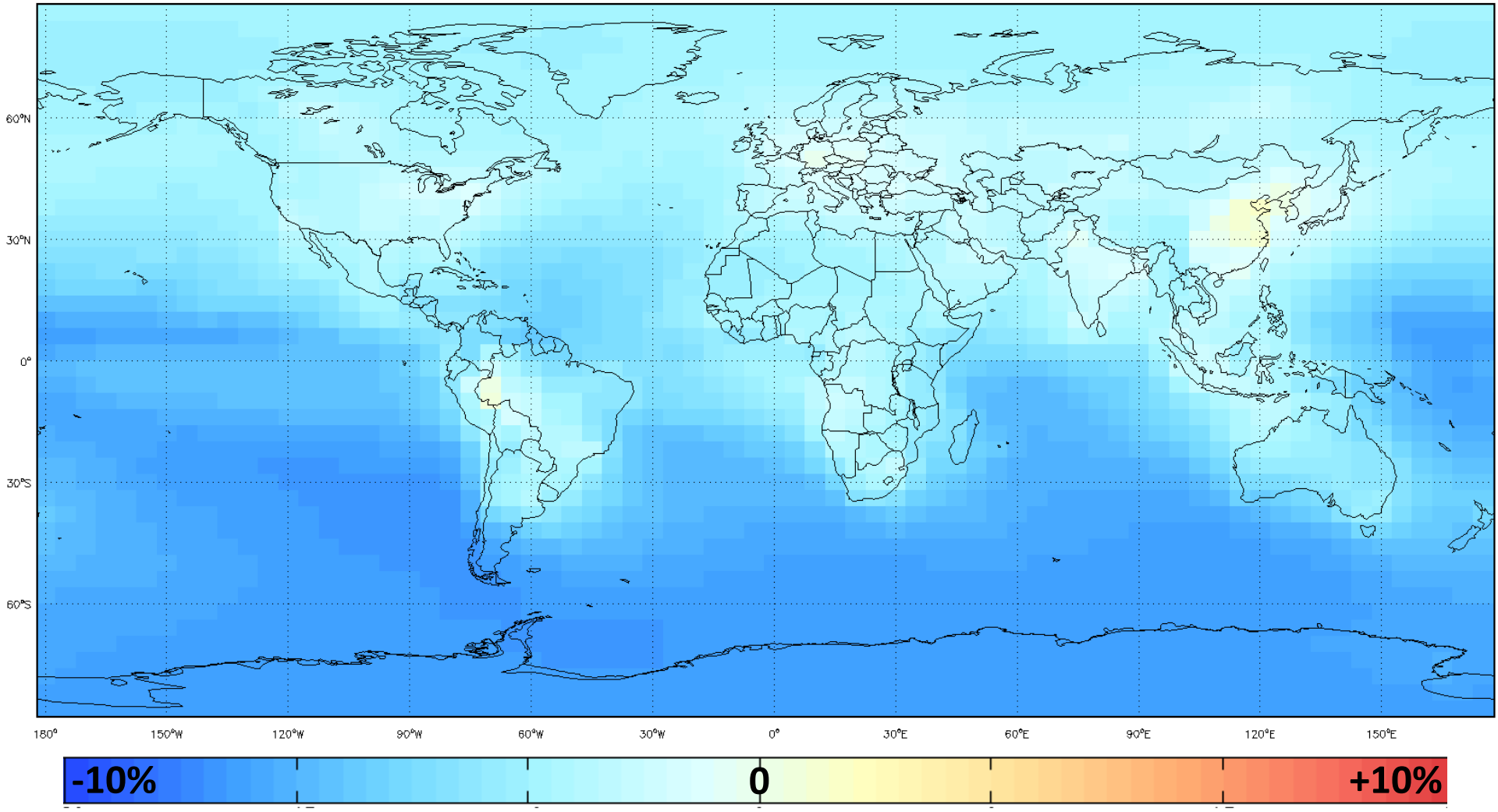
% change in [NO] at surface from old to new isoprene mechanism, 2014



Overall: Production ↓ 0.9%, Loading ↓ 1.4% (1km), 2.6% (atm)

Preliminary Results: Δ O_3

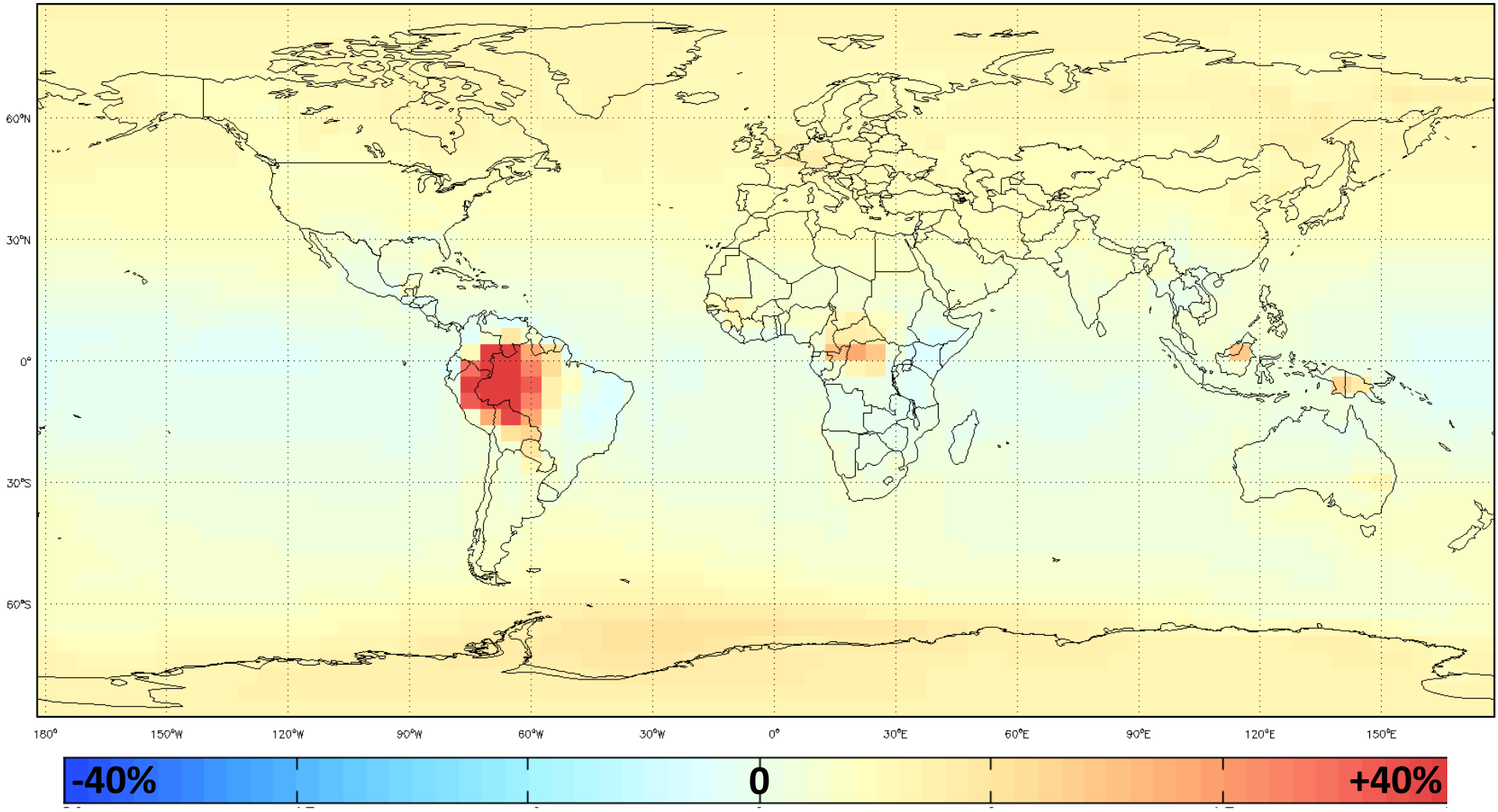
% change in [O_3] at surface from old to new isoprene mechanism, 2014



Overall: Production ↓ 2.3%, Loading ↓ 4.1% (1km), 7.2% (atm)

Preliminary Results: Δ OH

% change in [OH] at surface from old to new isoprene mechanism, 2014



Overall: Loading ↑ 2.7% (1km), ↓ 0.8% (atm)

Preliminary Results:

- Better representation of branching ratios for isomers and reactive pathways
- VOCs: ↑ isomerization fraction; ↑ MVK/MACR ratio; better representation of SOA precursors
- NO_x: increased transport
- Oxidants: ↓ $[O_3]$; ↑ [OH] in remote areas
- Sensitivity: $\partial[O_3]/\partial NO$ and $\partial[O_3]/\partial Isop$ skew positive