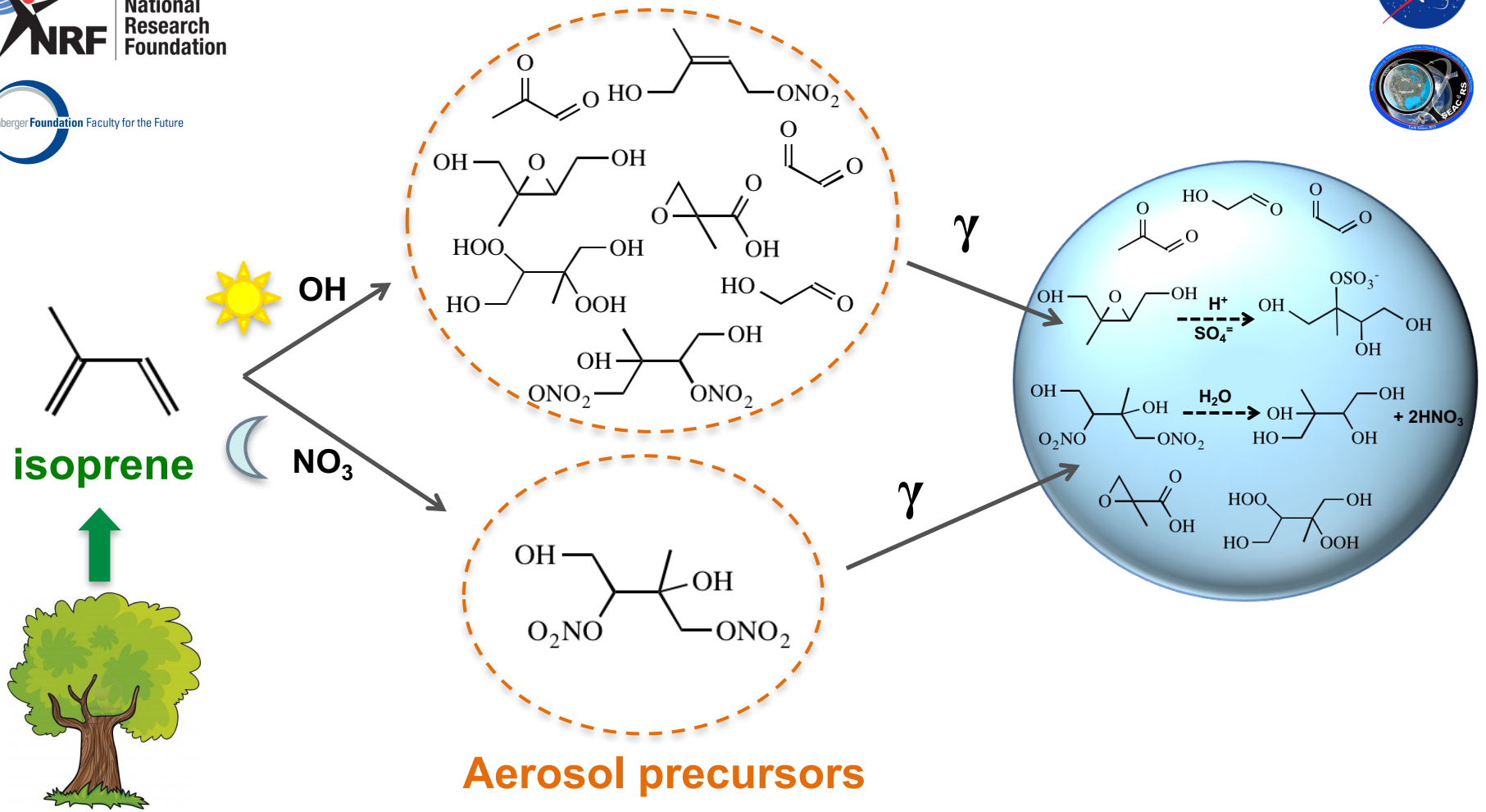
Updated GEOS-Chem Isoprene Secondary Organic Aerosol Mechanism



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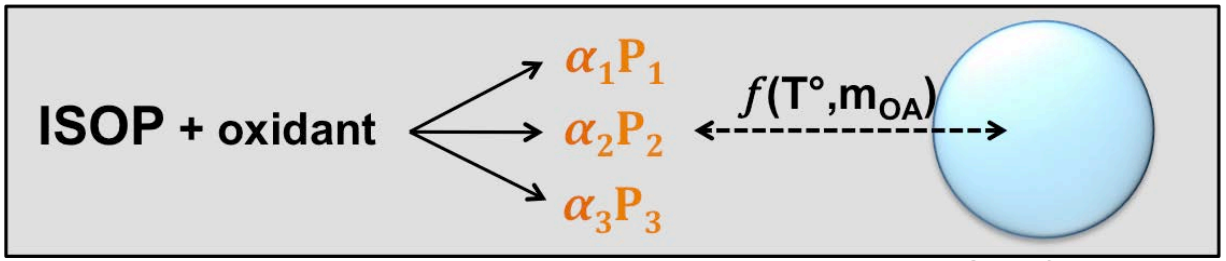
IGC7
Cambridge, MA
5 May 2015

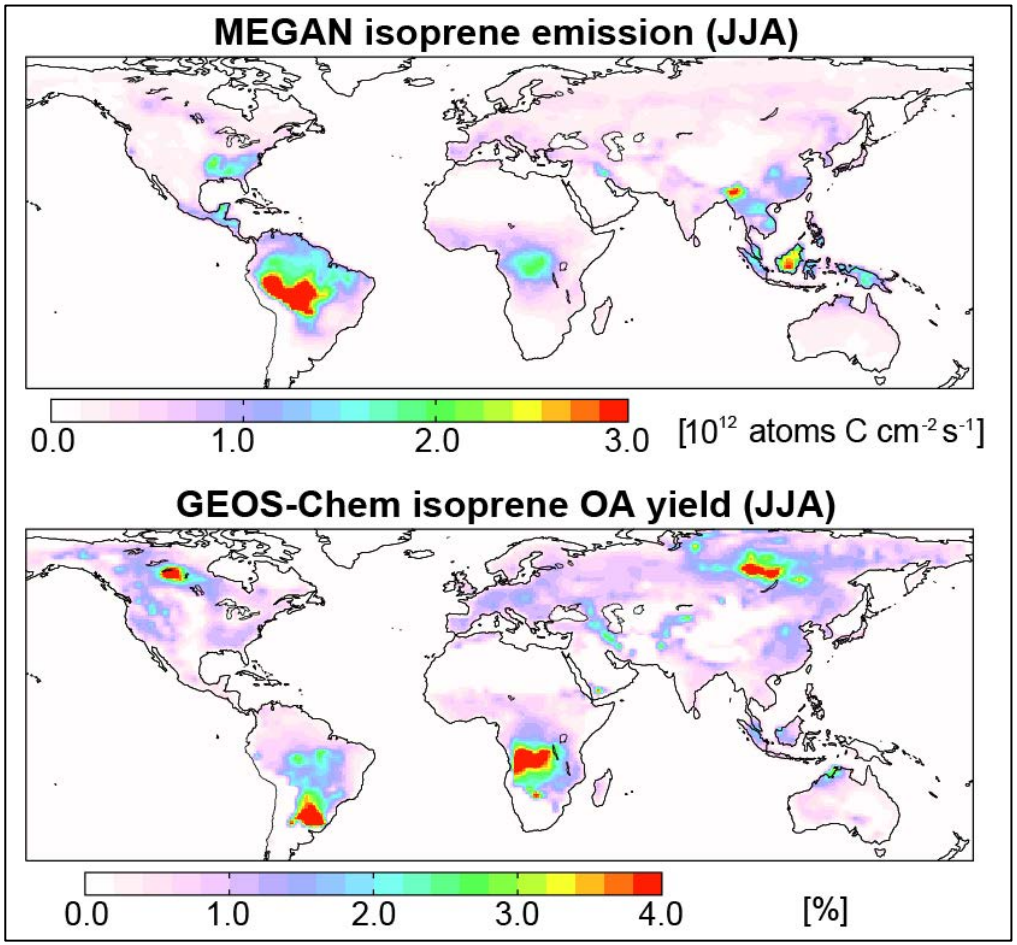
Default decoupled GEOS-Chem isoprene SOA scheme



[Pye and Seinfeld, 2010]

α: Gas-phase yield
P: Aerosol precursor
T°: temperature
$\mathbf{m_{OA}}$: pre-existing OA mass

Isoprene Emissions and isoprene aerosol yields are not collocated



Isoprene organic aerosol mass yield:

$$\text{Yield} = \frac{\Delta \text{SOA}_{\text{net}}}{\Delta \text{isoprene}}$$

Very low yields (**~1%**) in the southeast US and tropics

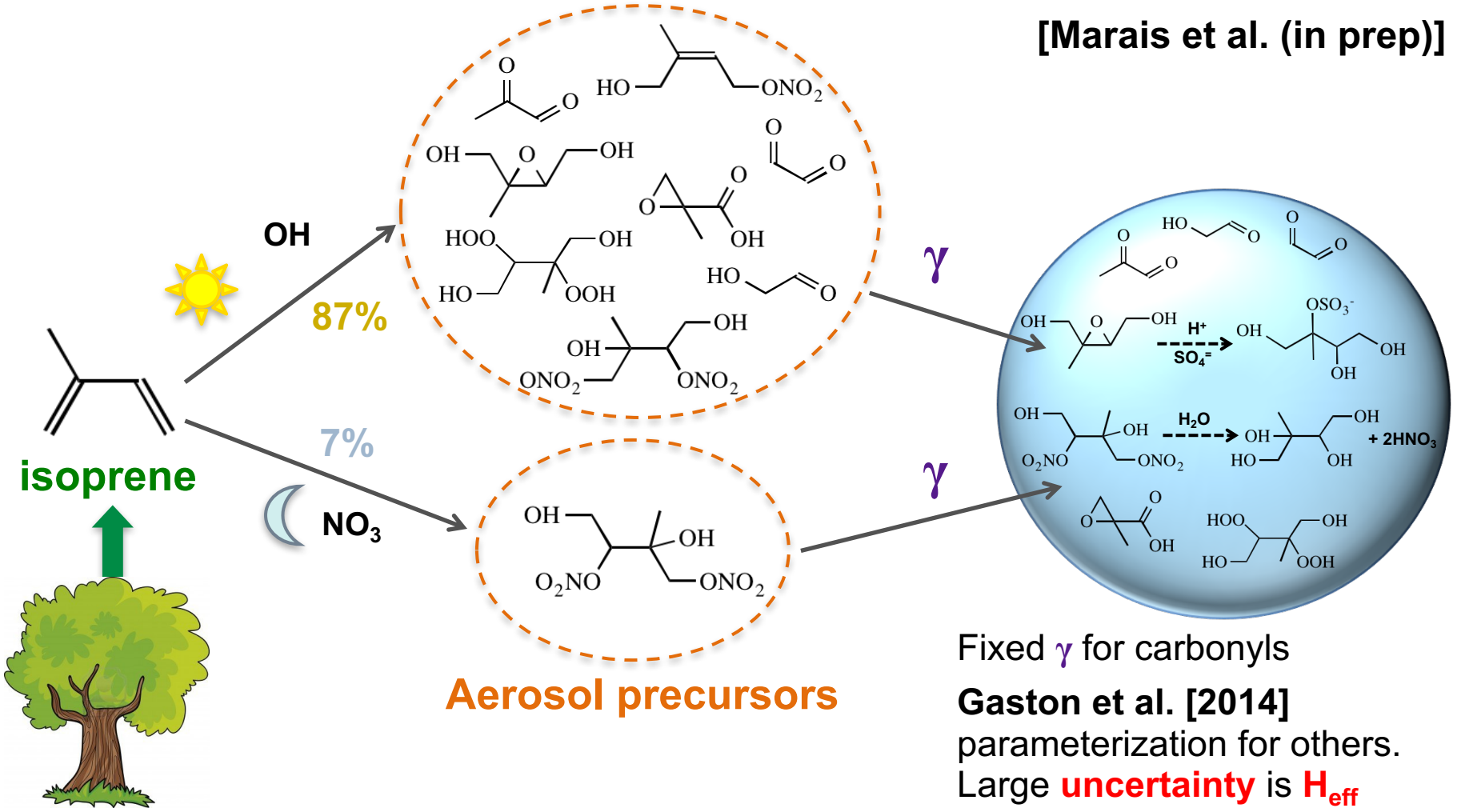
High yields where there is biomass burning (high pre-existing aerosol; low temperatures).

New GEOS-Chem isoprene SOA parameterization

Develop a mechanism that couples gas and aerosol phases

Better understand the processes that lead to isoprene SOA formation

[Marais et al. (in prep)]



Fixed γ for carbonyls

Gaston et al. [2014] parameterization for others.

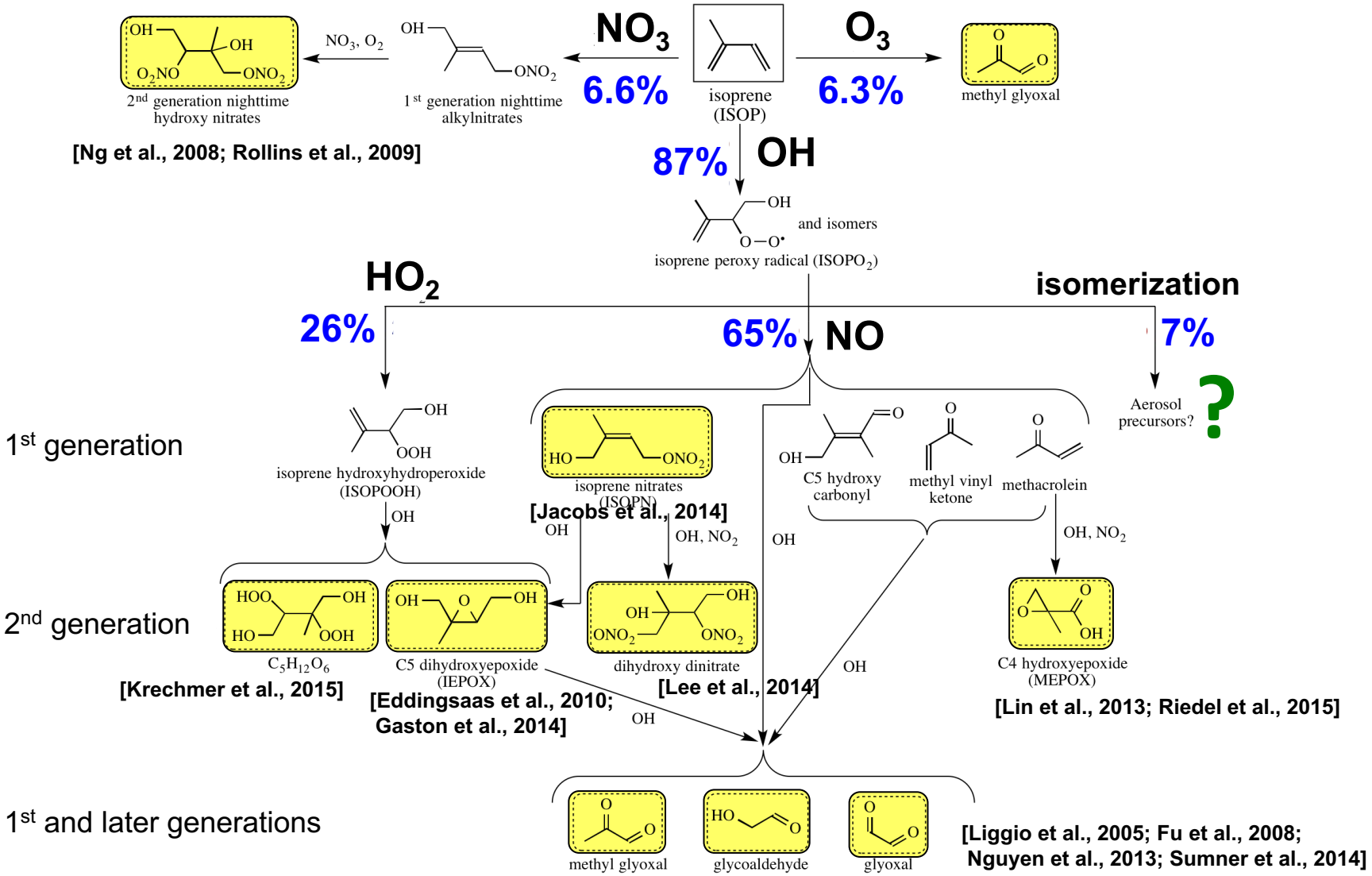
Large **uncertainty** is H_{eff}

Reversible partitioning of semivolatile precursors **retained for ISOP+OH** and **removed for ISOP+NO_3**

Isoprene OA precursors in GEOS-Chem

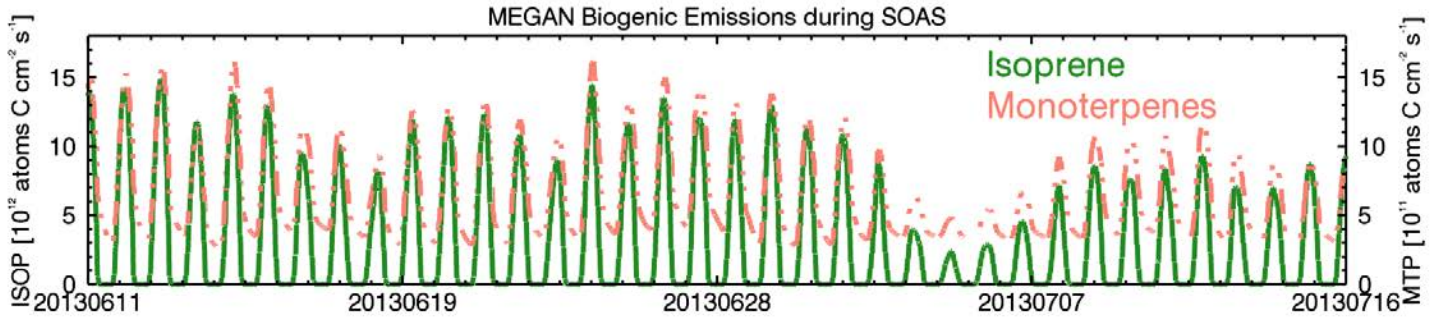
GEOS-Chem branching ratios:
Southeast US (Jun-Aug)

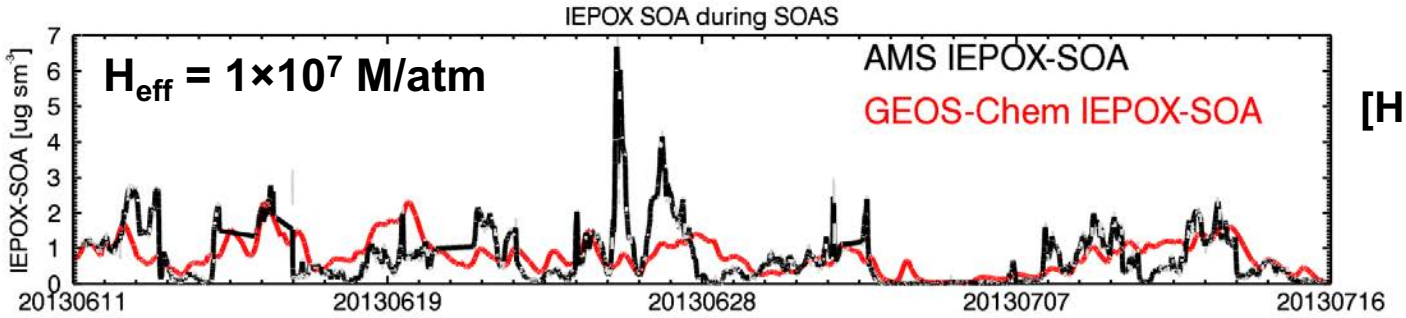
Aerosol precursors



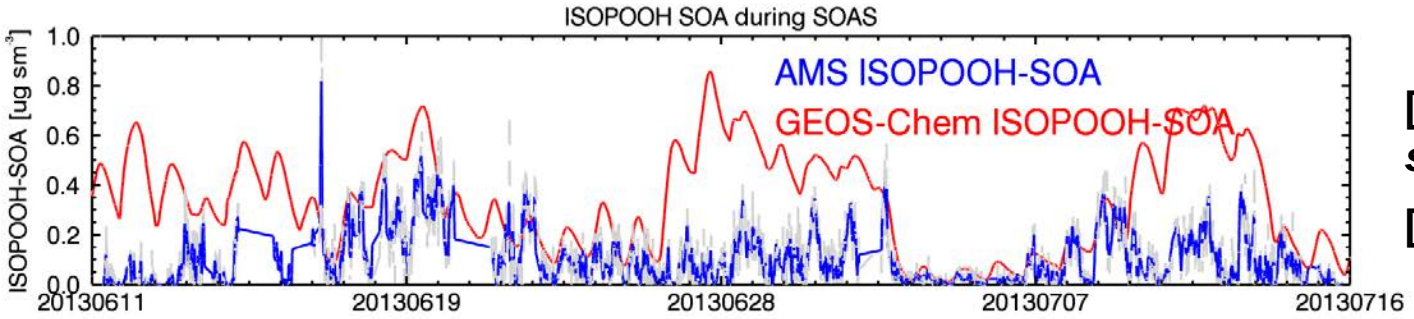
SOAS AMS and GEOS-Chem isoprene OA

Timeseries of MEGAN biogenic emissions, and GEOS-Chem and AMS IEPOX-SOA and ISOPOOH-SOA (Centreville, AL)





[Hu et al., ACPD, 2015]



[Krechmer et al., *submitted*, 2015]

[Liu et al (in prep)]

IEPOX-SOA is ~2 µg m^{-3} during SOAS. ISOPOOH-SOA is an order of magnitude lower.

GEOS-Chem captures temporal variability during SOAS. GEOS-Chem IEPOX-SOA sensitive to effective Henry's constant (H_{eff})

Concluding Remarks

- New isoprene scheme couples the gas and aerosol phase chemistry in GEOS-Chem.
- Aerosol precursors uptake now represents a loss pathway.
- GEOS-Chem IEPOX-SOA and ISOPOOH-SOA temporal variability is consistent with the SOAS surface measurements in Centreville, AL.

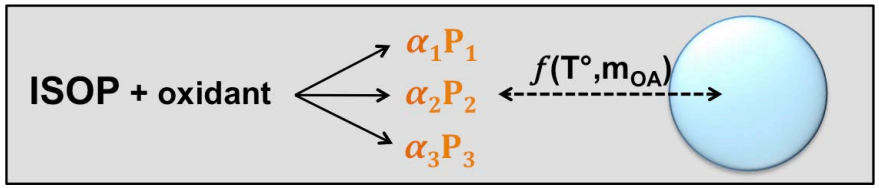
Next Steps

- Add aerosol-phase formation of methyltetrols and organosulfates from IEPOX-SOA
- Derive isoprene SOA yields with global satellite column HCHO retrievals and surface/aircraft aerosol mass spectrometer measurements.
- Replace default monoterpene SOA scheme with similar mechanistic representation of monoterpene SOA formationm

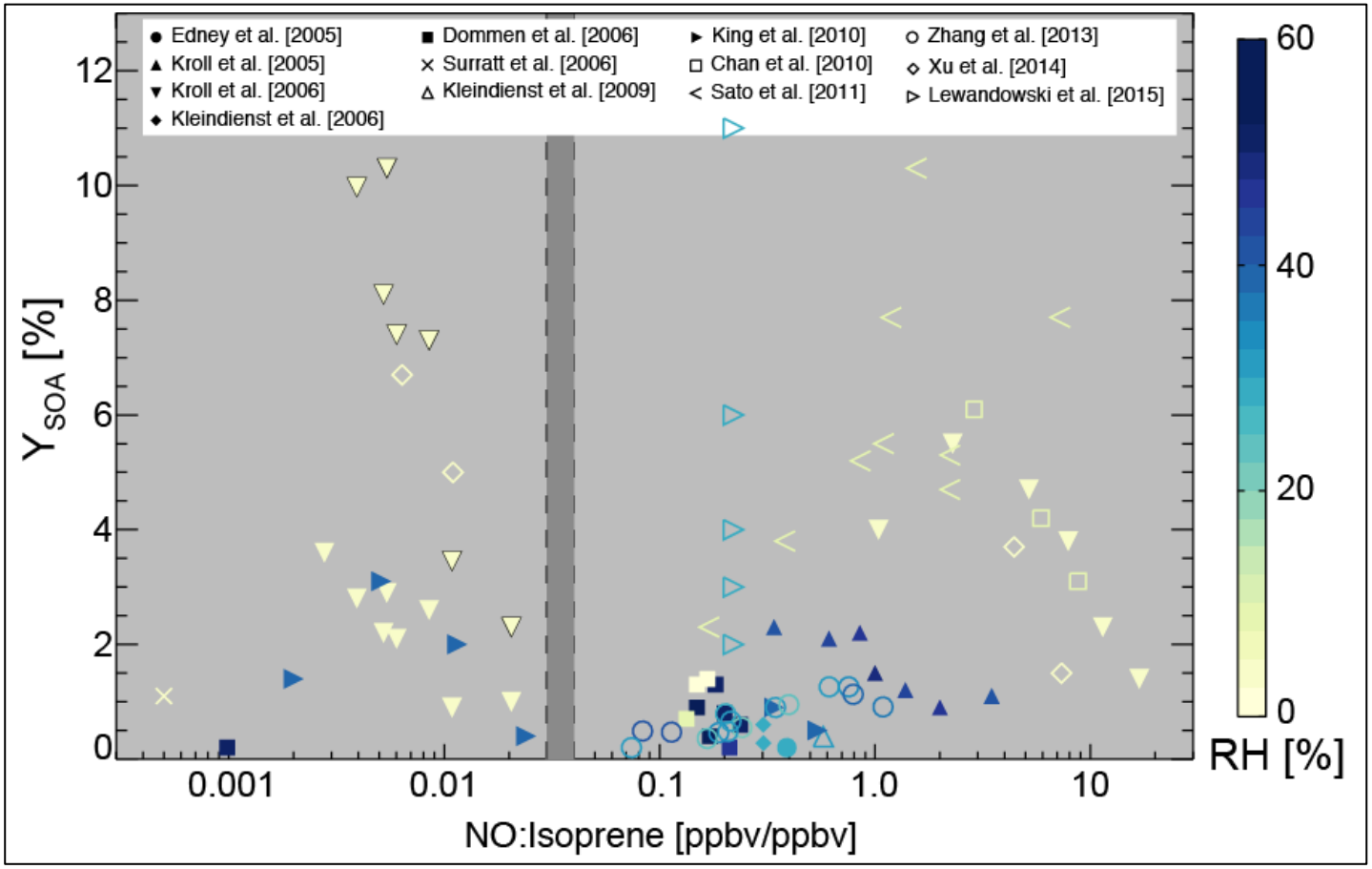
Supplementary Slides

GEOS-Chem uses fixed yields of gas-phase SOA precursors from chamber studies

Default isoprene SOA scheme:



Use fixed yields (α_i), despite large variability in **chamber studies**:



Lab results for **OA < 20 µg m^{-3}**

Yields colored by **relative humidity**

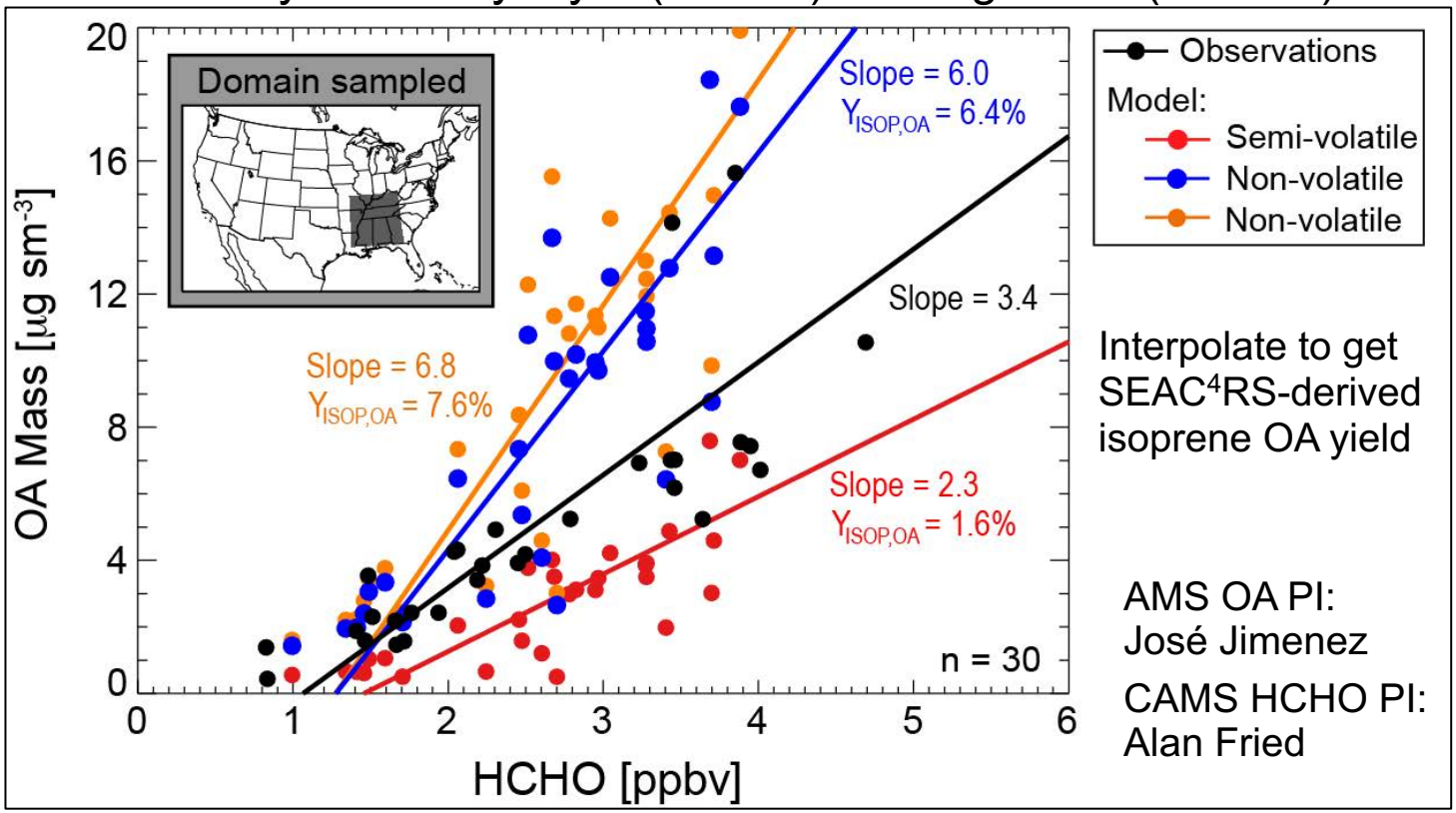
In GEOS-Chem **α_i is ~3% at 10 µg m^{-3}**.

Realized yields are lower

SEAC⁴RS-derived isoprene OA yields

OA-HCHO relationship during SEAC⁴RS

Points are daily boundary-layer (< 2 km) mean gridded (2°×2.5°) data



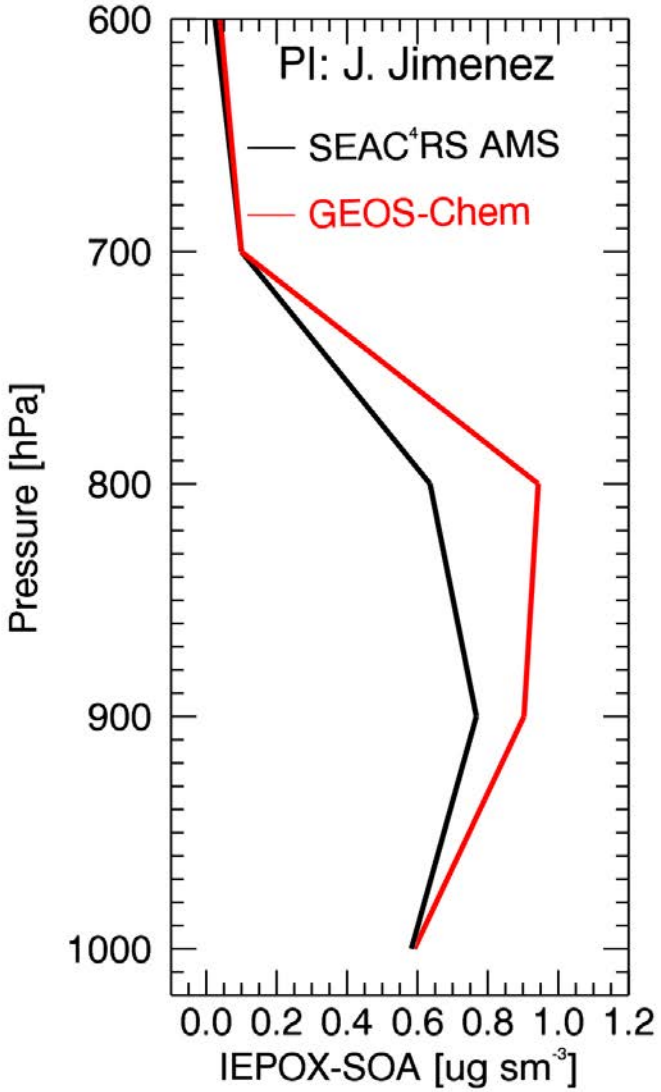
By interpolation, SEAC⁴RS-derived **isoprene OA yield is 3 %**

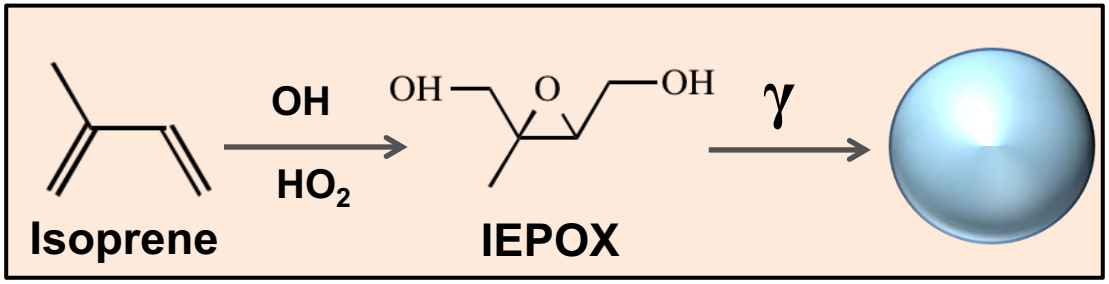
SEAC⁴RS OA -HCHO relationship provides total isoprene SOA yields.

Obtain additional information from AMS-derived isoprene SOA components

GEOS-Chem isoprene OA during SEAC^{4}RS

Vertical profile of AMS-derived IEPOX-SOA and GEOS-Chem IEPOX-SOA





Relatively uniform distribution throughout the boundary layer

Slight model overestimate likely caused by gas-phase overestimate in IEPOX, but also likely due to uncertain uptake dynamics.

IEPOX-SOA data provided by P. Campuzano-Jost