



# Modeling regional air quality using the near-explicit Master Chemical Mechanism (MCM)

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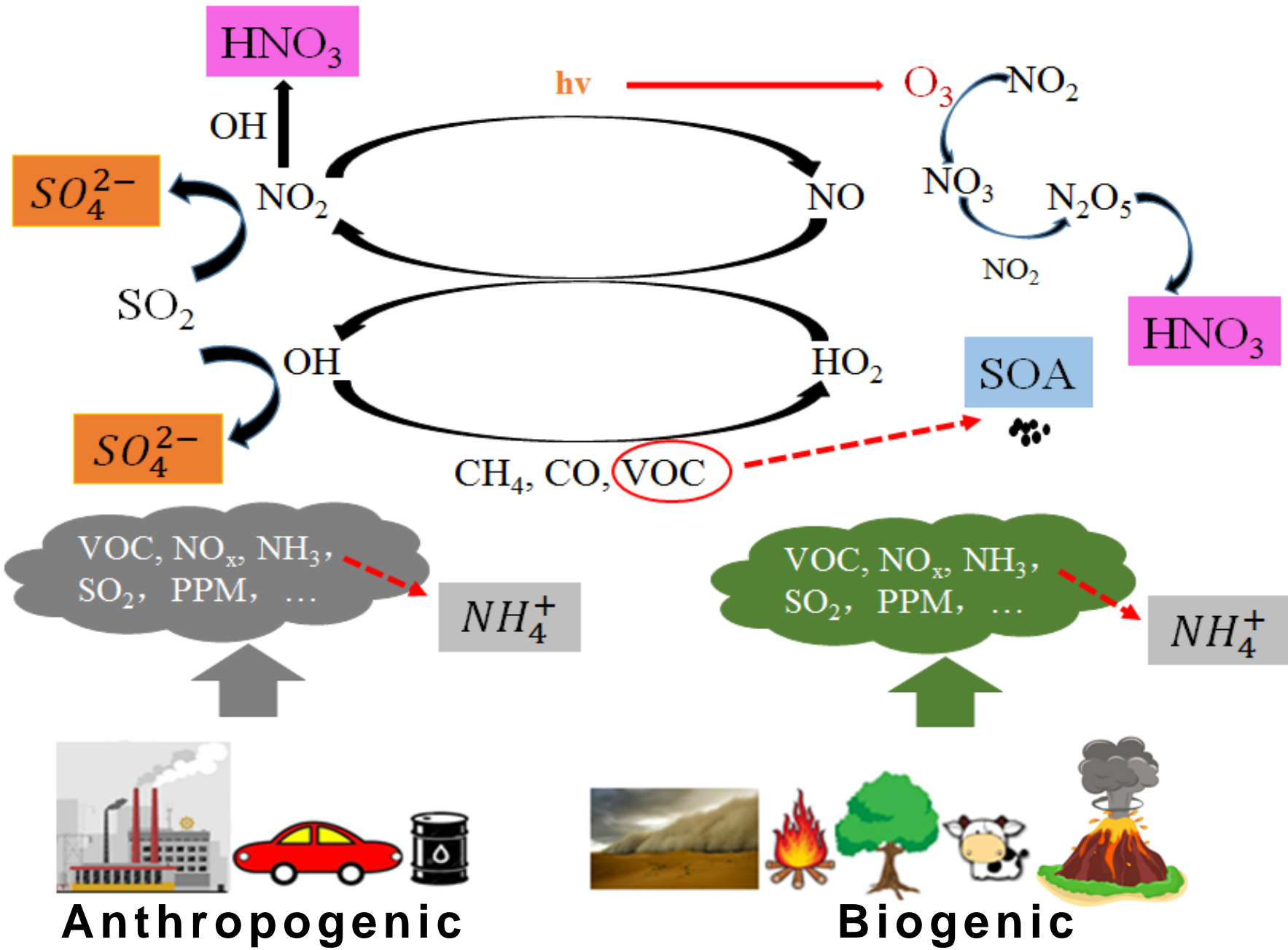
Funding from NSFC

The 1<sup>st</sup> Regional GEOS-Chem Asia Meeting

# Outline

- Motivations
- Application of CMAQ-MCM-SOA in simulating regional air quality over the eastern U.S.
- Future studies in China

# Ozone and PM<sub>2.5</sub> are correlated by the precursors

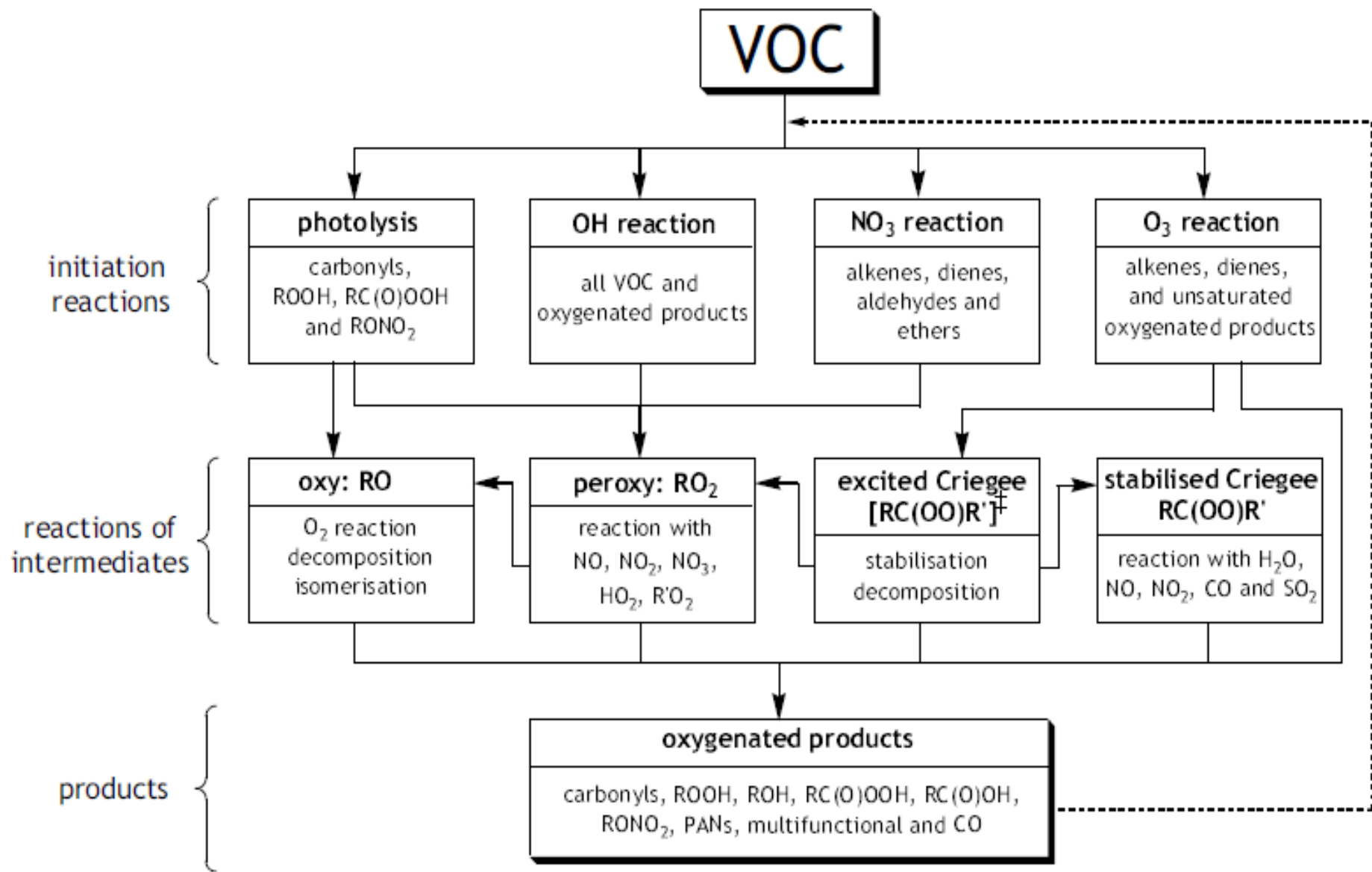


- Biases in estimates of ozone and PM<sub>2.5</sub> from Air Quality Models (AQMs)
  - Uncertainties in emission inventories (especially VOCs)
  - Complicated gas- and particle-phase chemistry
  - Representation of mass transfer of semi volatile organic compounds (SVOCs) gas-phase ↔ particle-phase

**Nonlinearity of ozone-PM<sub>2.5</sub>-VOCs/NO<sub>x</sub> is not well understood**

# Why MCM?

142 primary emitted VOCs



(Saunders et al., 2003)

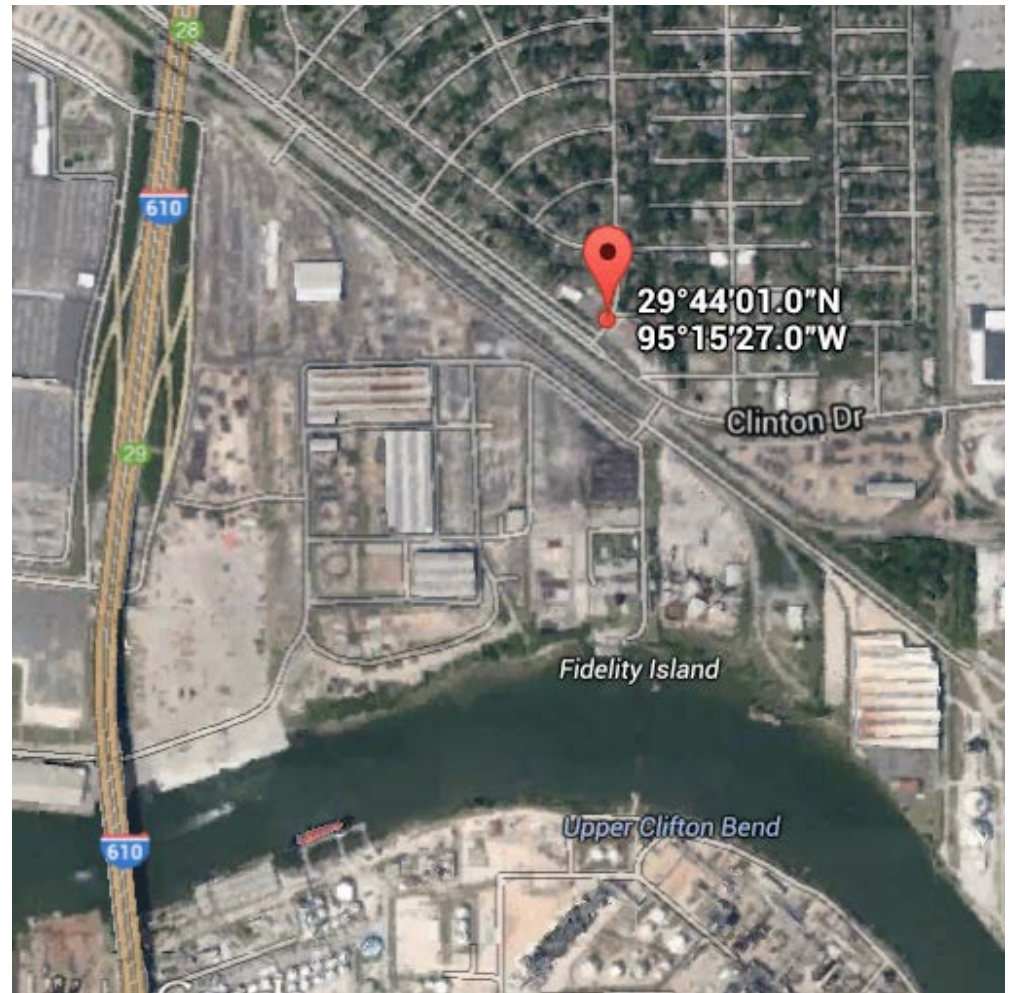
# Why MCM?

- Uncertainties in emission inventories of VOCs ?
  - compare the predicted concentration of each primary VOC with observations
- Complicated gas- and particle-phase chemistry?
  - update and apply MCM to a regional AQM
- Representation of gas-phase ↔ particle-phase for SVOCs?
  - equilibrium partitioning of SVOCs
  - reactive uptake of dicarbonyls, isoprene epoxydiols (IEPOX), and methacrylic acid epoxide (MAE)

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# VOC prediction @ Clinton Drive (C35C)



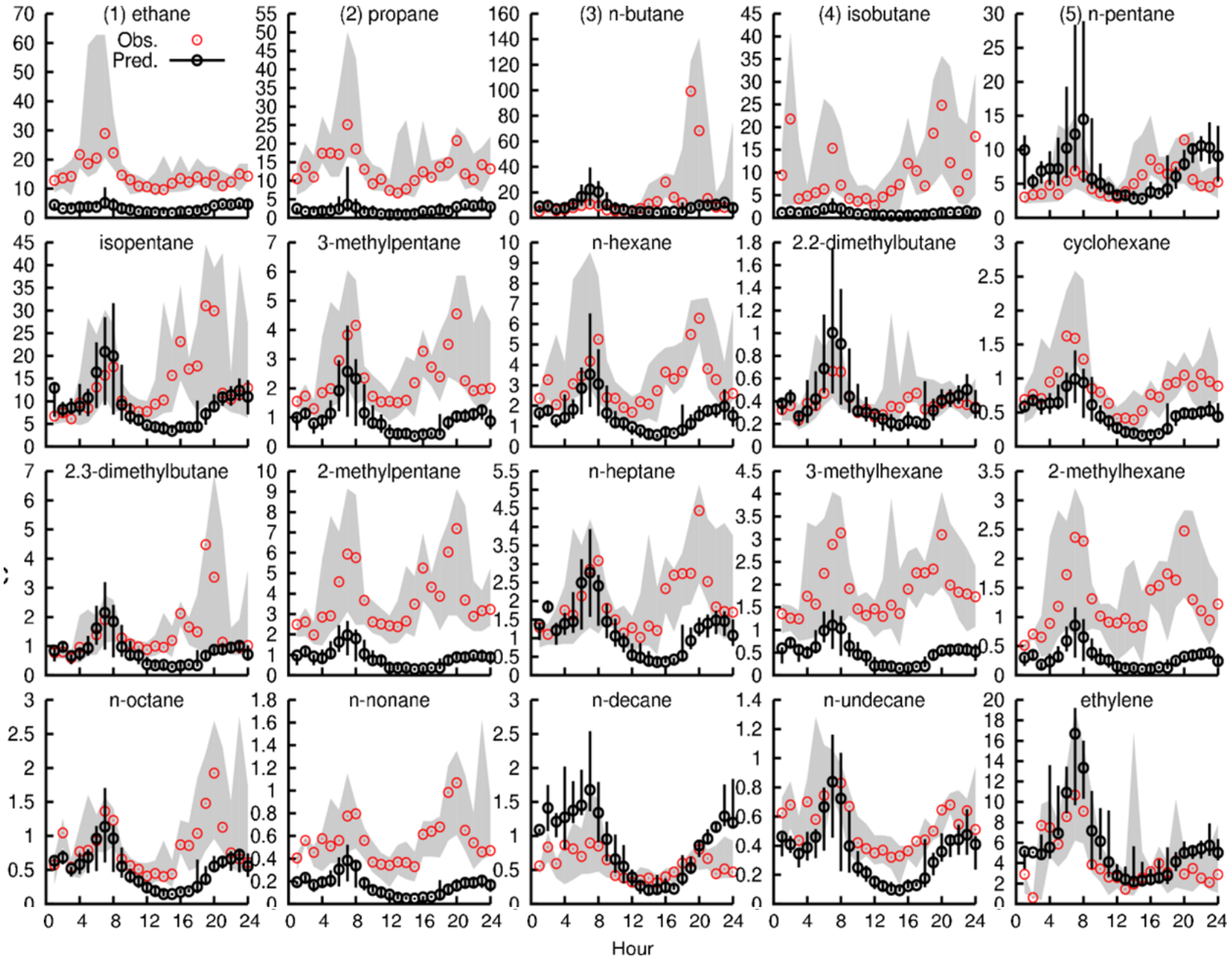
August 16-September 6, 2000

(Ying and Li, 2011)

Obs. 25<sup>th</sup>-75<sup>th</sup>

Pred. 25<sup>th</sup>-75<sup>th</sup>

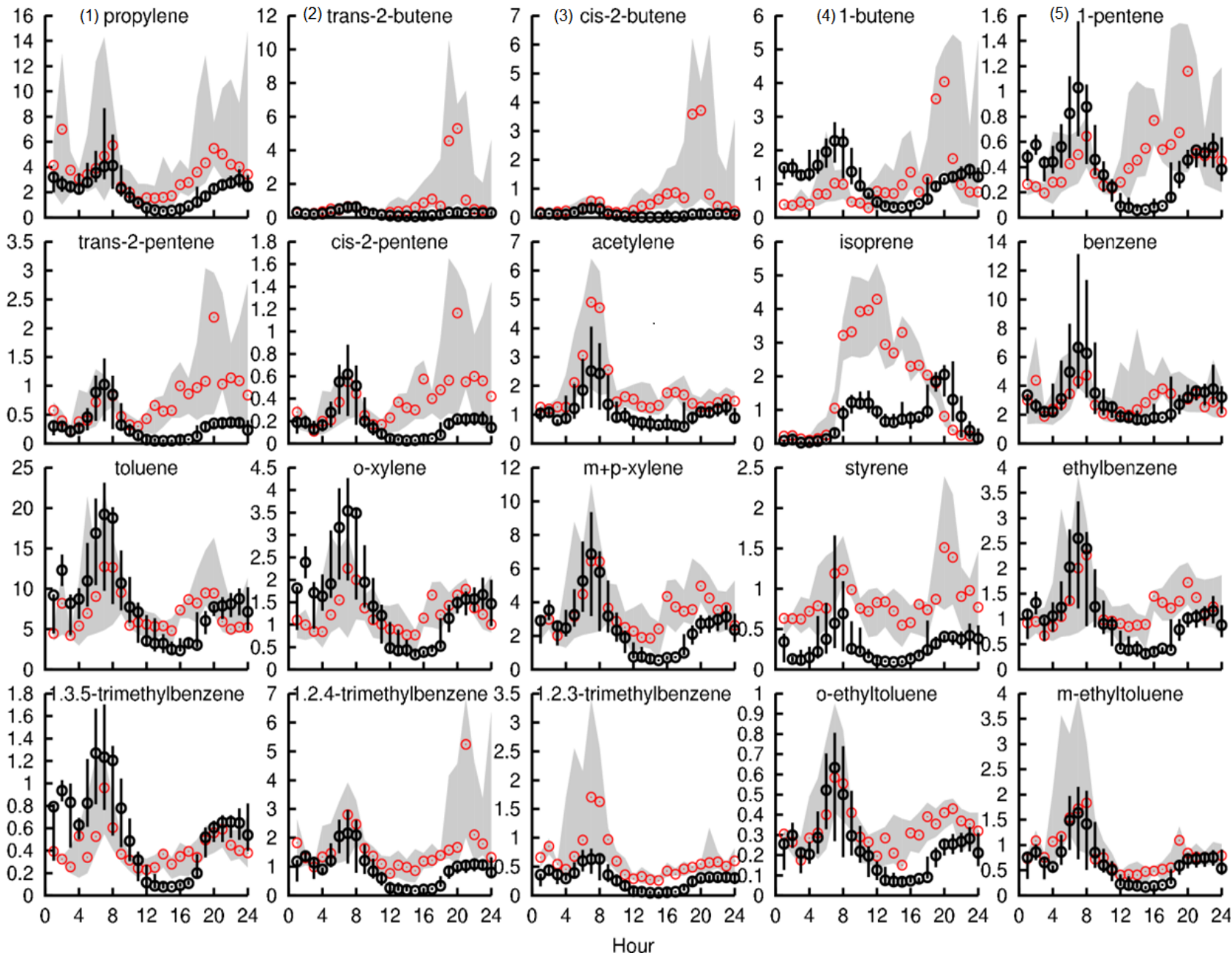
Units: ppbC



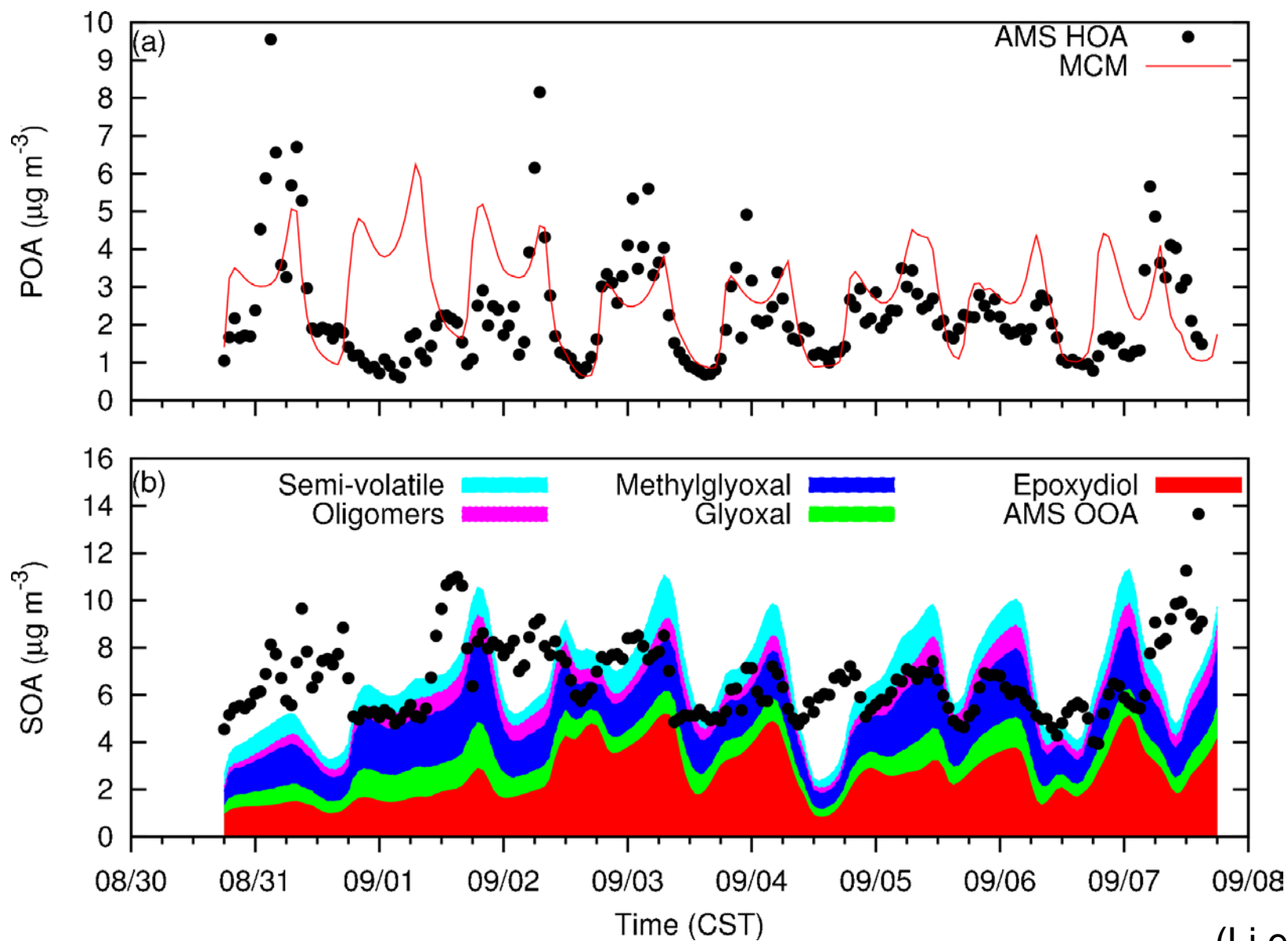
Obs. 25<sup>th</sup>-75<sup>th</sup>

Pred. 25<sup>th</sup>-75<sup>th</sup>

Units: ppbC



# Aerosols at Moddy Tower, UH

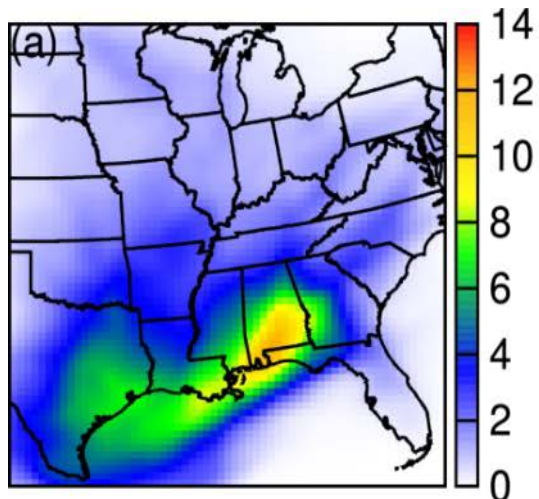


(Li et al., 2015)

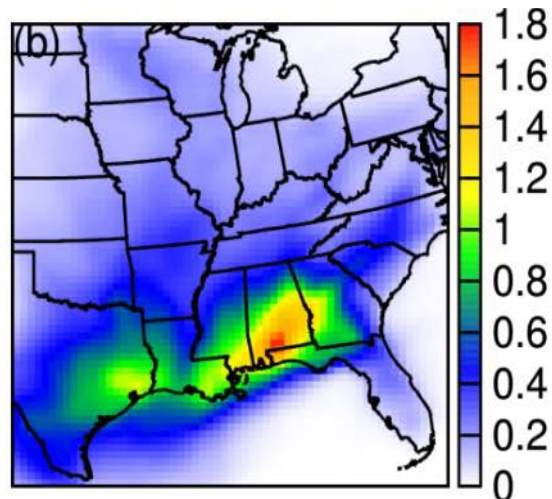
# SOA components

Units:  $\mu\text{g}/\text{m}^3$

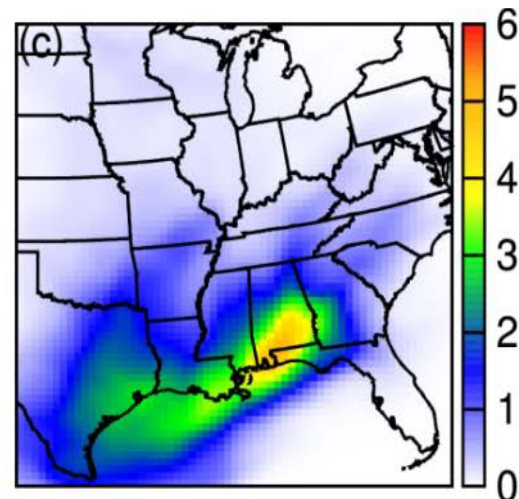
Total SOA



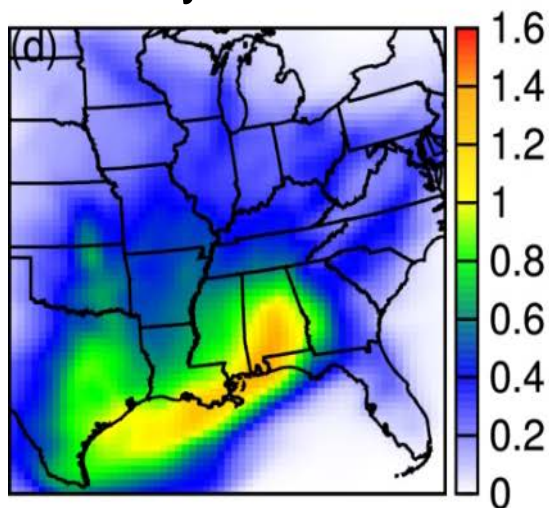
Semi-volatile SOA



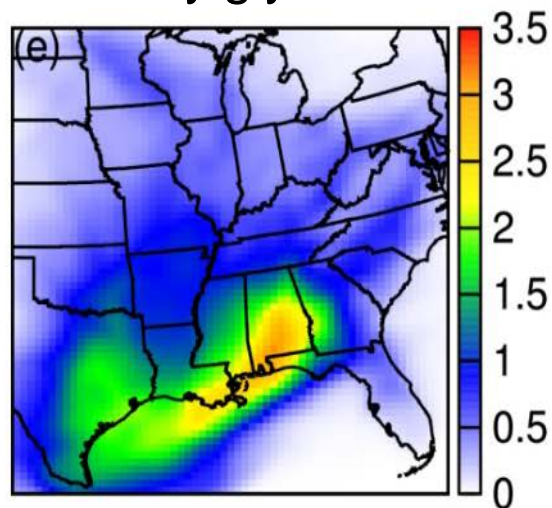
IEPOX+MAE



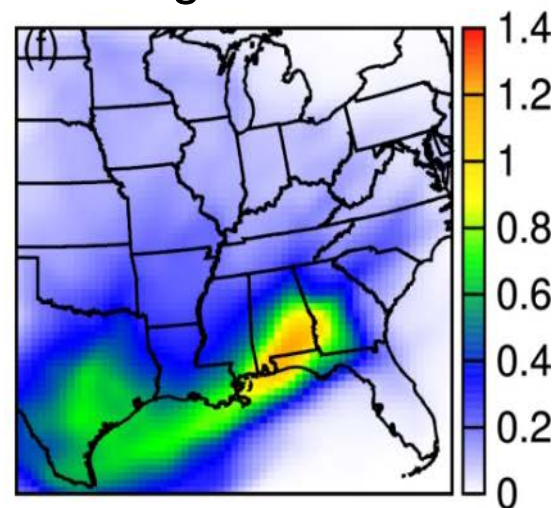
Glyoxal



Methylglyoxal



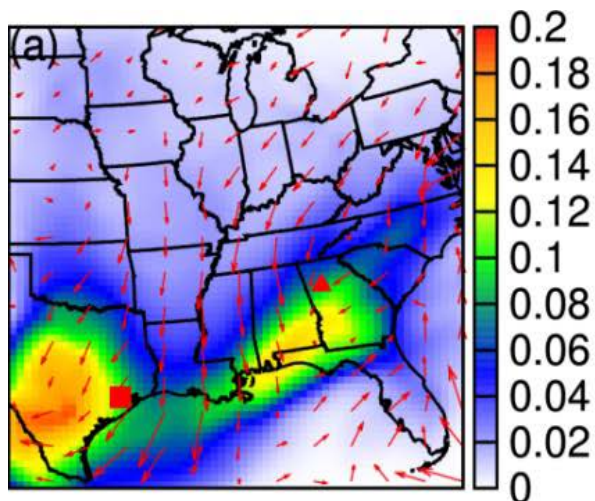
Oligomers



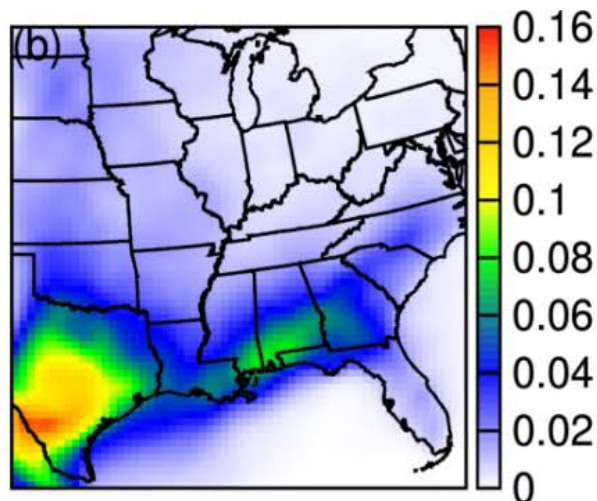
# Major SVOCs (column total conc.)

Units: mg/m<sup>2</sup>

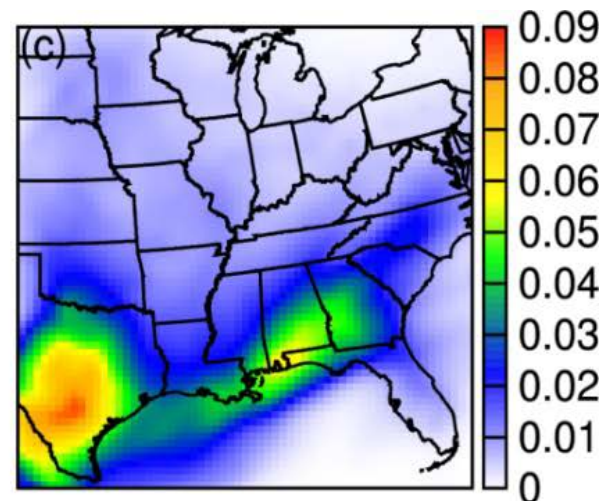
$\beta$ -caryophyllene



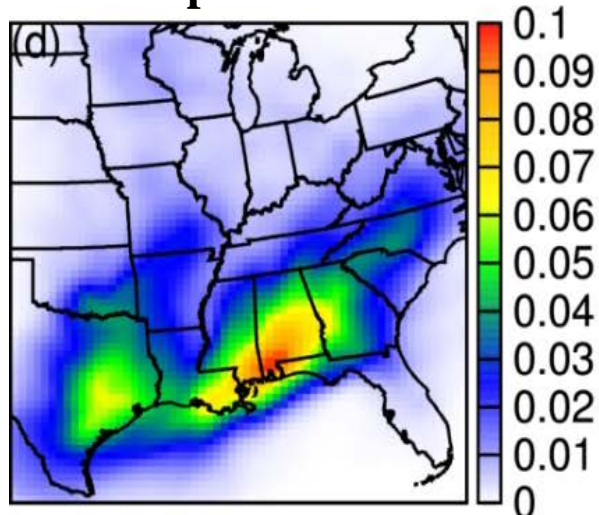
$\beta$ -caryophyllene



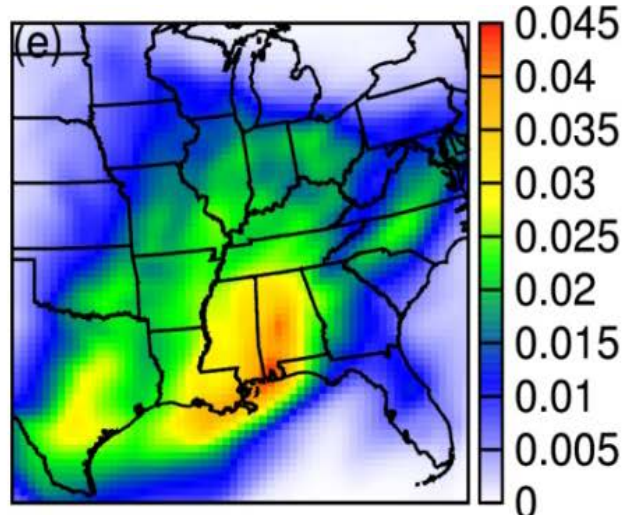
$\beta$ -caryophyllene



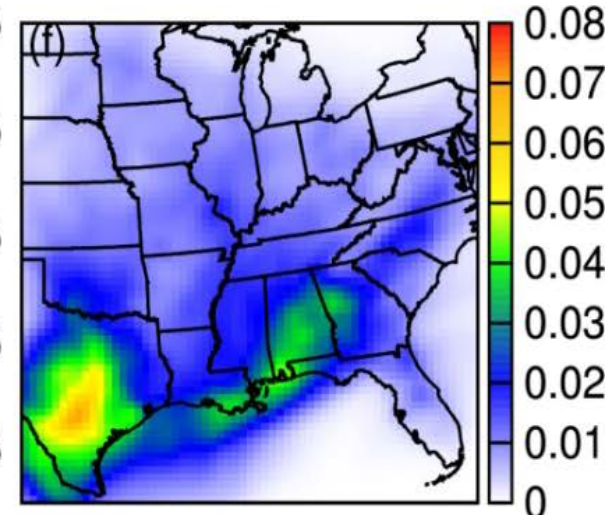
isoprene



toluene



$\beta$ -caryophyllene



→ Wind field

■ Houston

▲ Atlanta

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# What to do?

- Emission inventory of VOCs from different sources (speciation of total VOCs)
- Improvements to the current model
  - ✓ MCMv3.3.1
  - ✓ Dynamic partitioning vs. equilibrium partitioning
  - ✓ Heterogeneous formation of sulfate and nitrate
  - ✓ Aqueous-phase chemistry for soluble organics
  - ✓ Updates in isoprene chemistry
- Responses of ozone and  $\text{PM}_{2.5}$  to the precursors

