Modeling oxidant chemistry in a high-isoprene atmospheric environment: sensitivity to model resolution and constraints from aircraft observations

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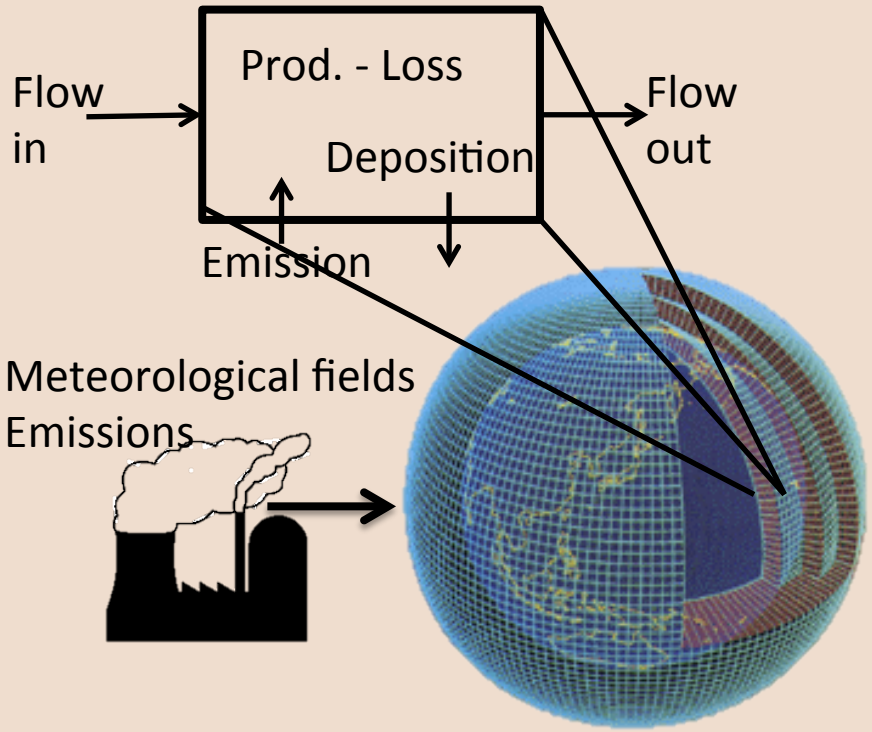
SEAC^{4}RS Science Team Meeting

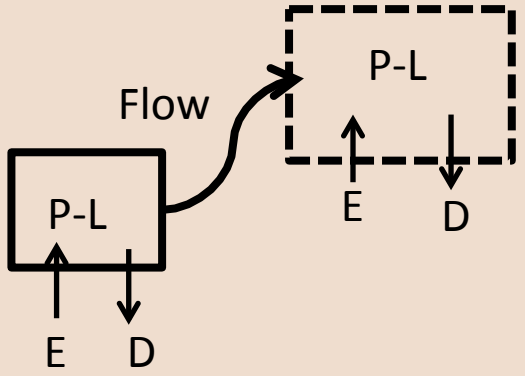
Global simulations of tropospheric chemistry represent a major computational challenge

Eulerian



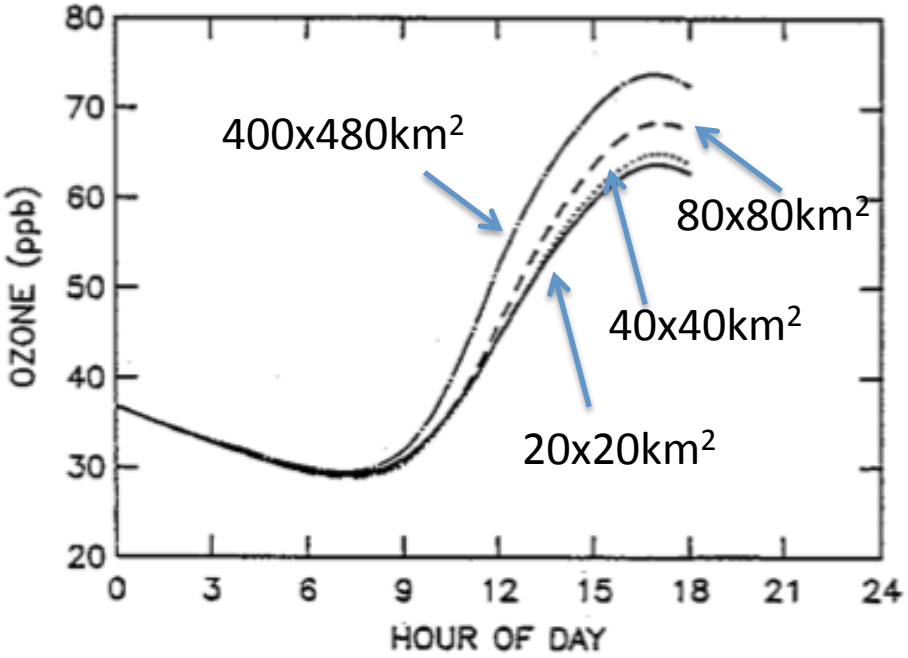
- Chemical mechanisms typically include >100 coupled species
- Chemical process interact with transport processes on wide range of scales

Lagrangian



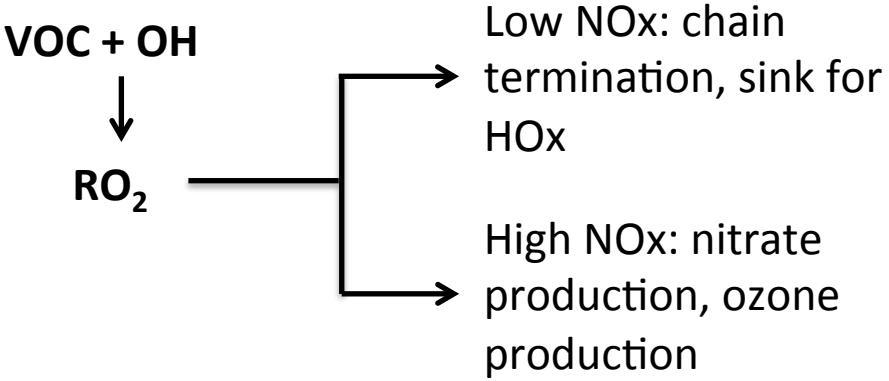
Resolution	Resource requirements (normalized to 4x5)
$4^o x 5^o$	1
$2^o x 2.5^o$	188
$0.25^o x 0.3125^o$	12032

Earlier work emphasized the effect of distributing NO_X emissions from urban regions into coarse grid cells



[*Sillman et al. (1990)*]

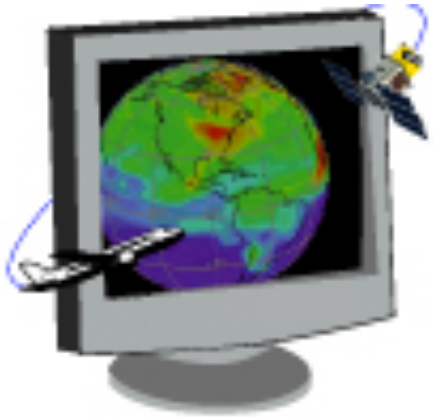
- Effect of grid resolution on NO_X-saturated vs. NO_X-limited regime has been extensively studied.
- As NO_X emissions decline, it becomes increasingly important to evaluate model ability to represent interaction of biogenic and anthropogenic emissions.



How does grid resolution affect model representation of high-NOx vs. low-NOx regimes?

Evaluate GEOS-Chem run at 4°x5°, 2°x2.5° and 0.25°x0.3125° resolutions against SEAC^{4}RS observations

GEOS meteorology at 0.25x0.3125 resolution

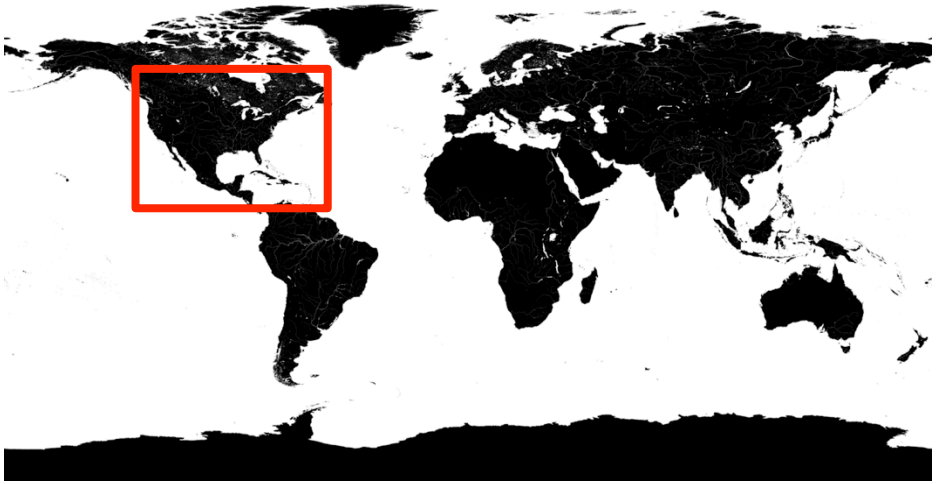


4x5 global, starting January 2013

2x2.5 global, start January 2013

0.25x0.3125 N. America with 4x5 boundary conditions, start run August 2013

Instrument (PI)	Measurement
CSD CL (T. Ryerson)	Ozone
	NO
	NO_2
PTRMS (A. Wisthaler)	Isoprene
CAMS (A. Fried)	Formaldehyde
CIT-CIMS (P. Wennberg)	ISOPN
	ISOPOOH



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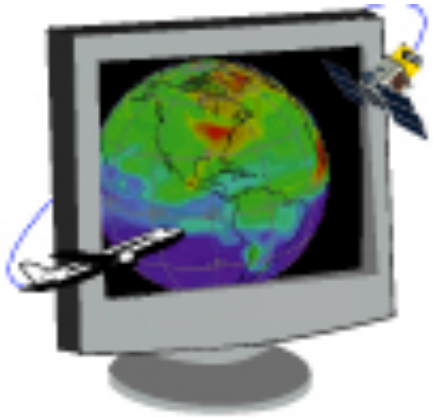

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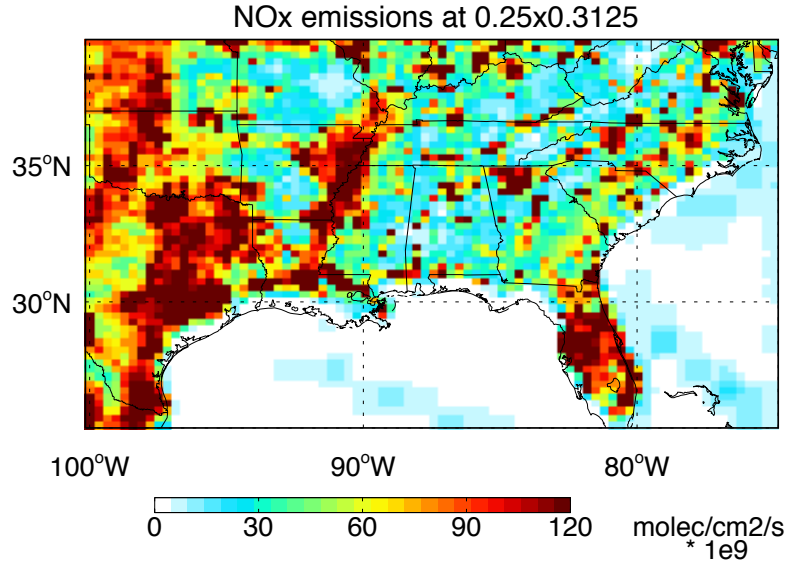
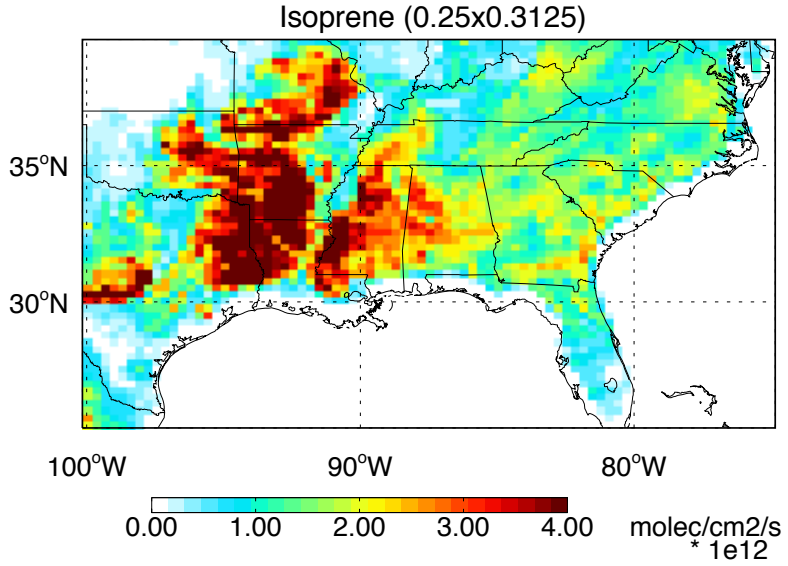
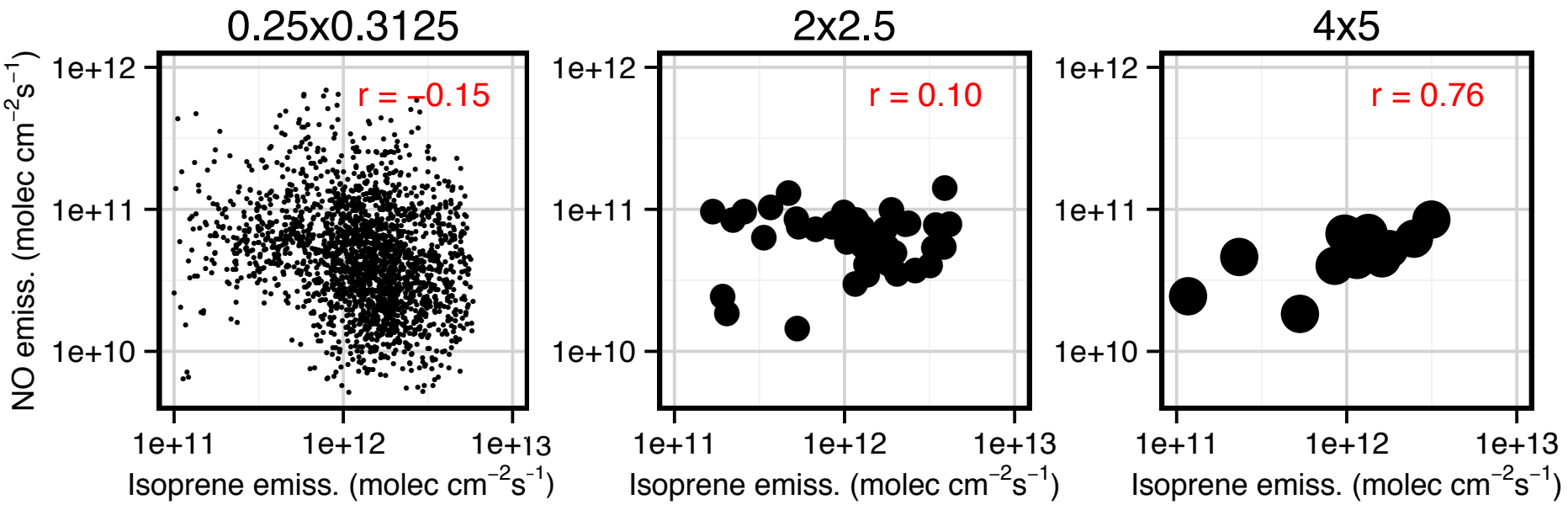
Boundary layer comparisons

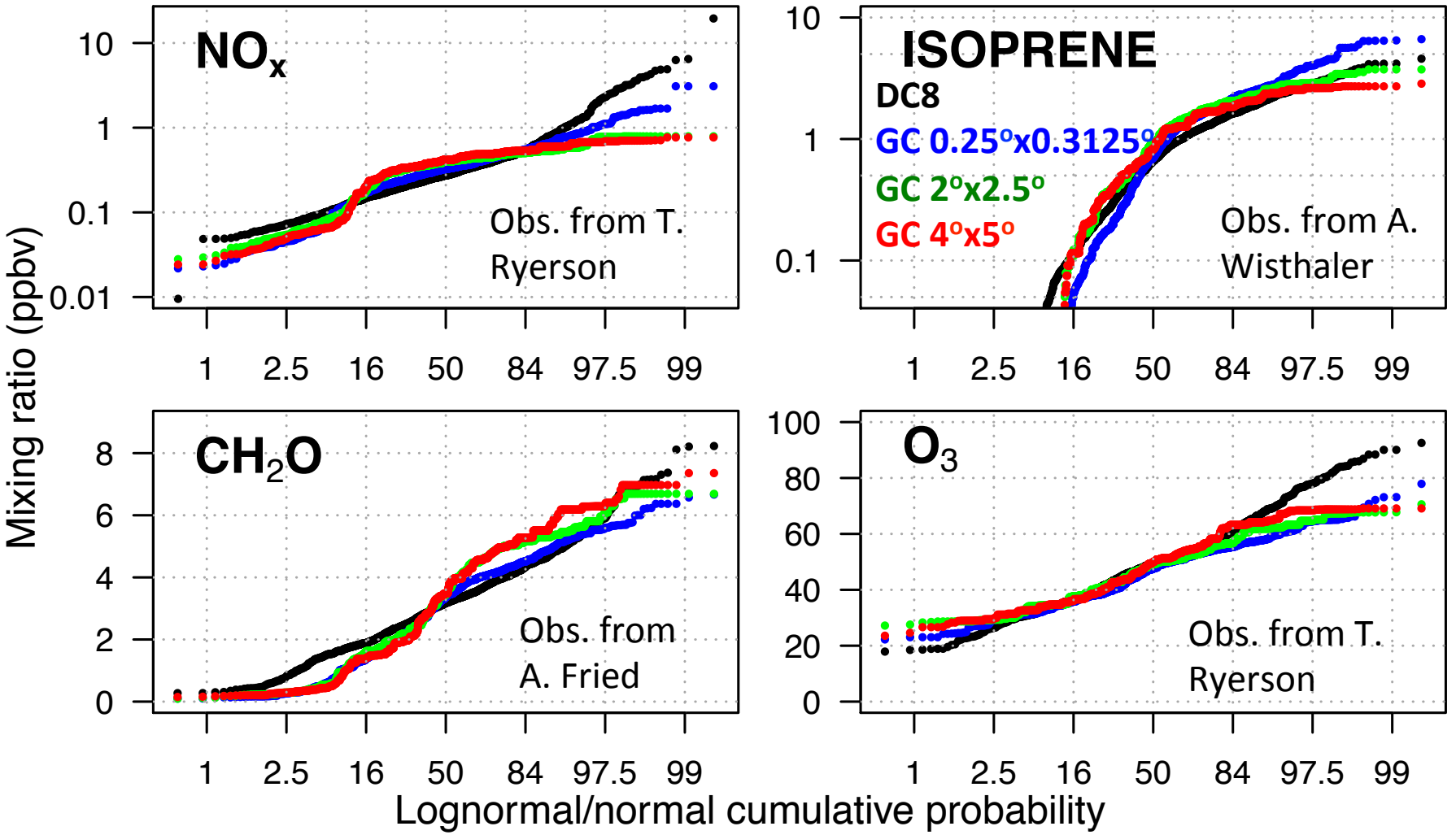
Emissions of NOx and isoprene in Southeast US show high granularity and spatial anti-correlation







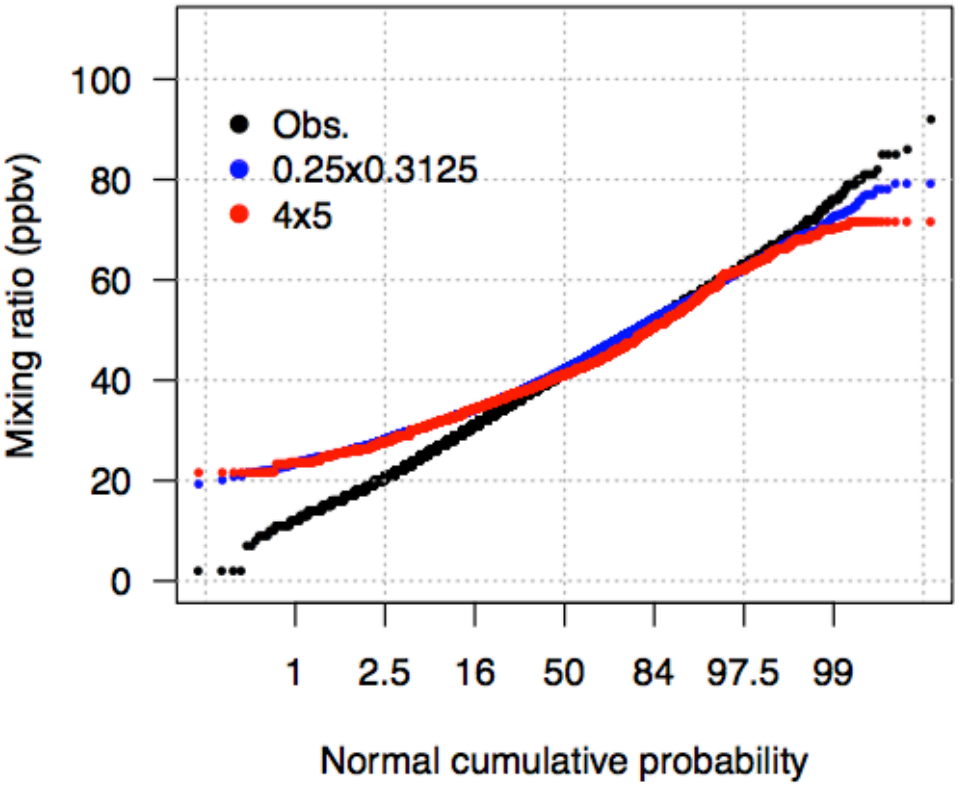
Probability distributions for primary and secondary species



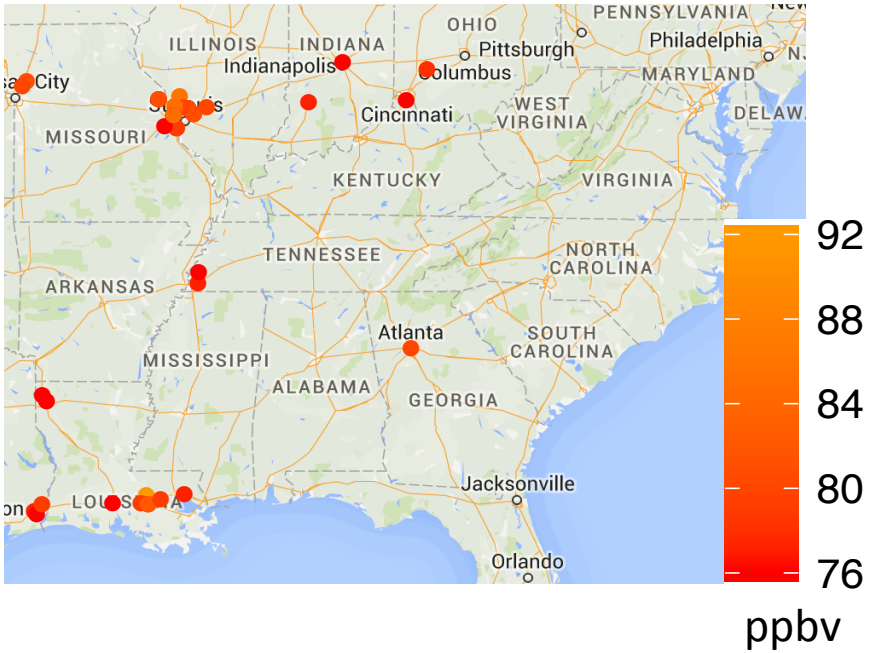
- Effect of grid resolution more apparent for highly skewed distributions: resolution of small-scale features allows for more extreme tail values
- Resolution differences for secondary species related to differences in chemical pathways

AQS surface measurements provide additional information on air quality in the Southeast US

MDA8 ozone at AQS sites

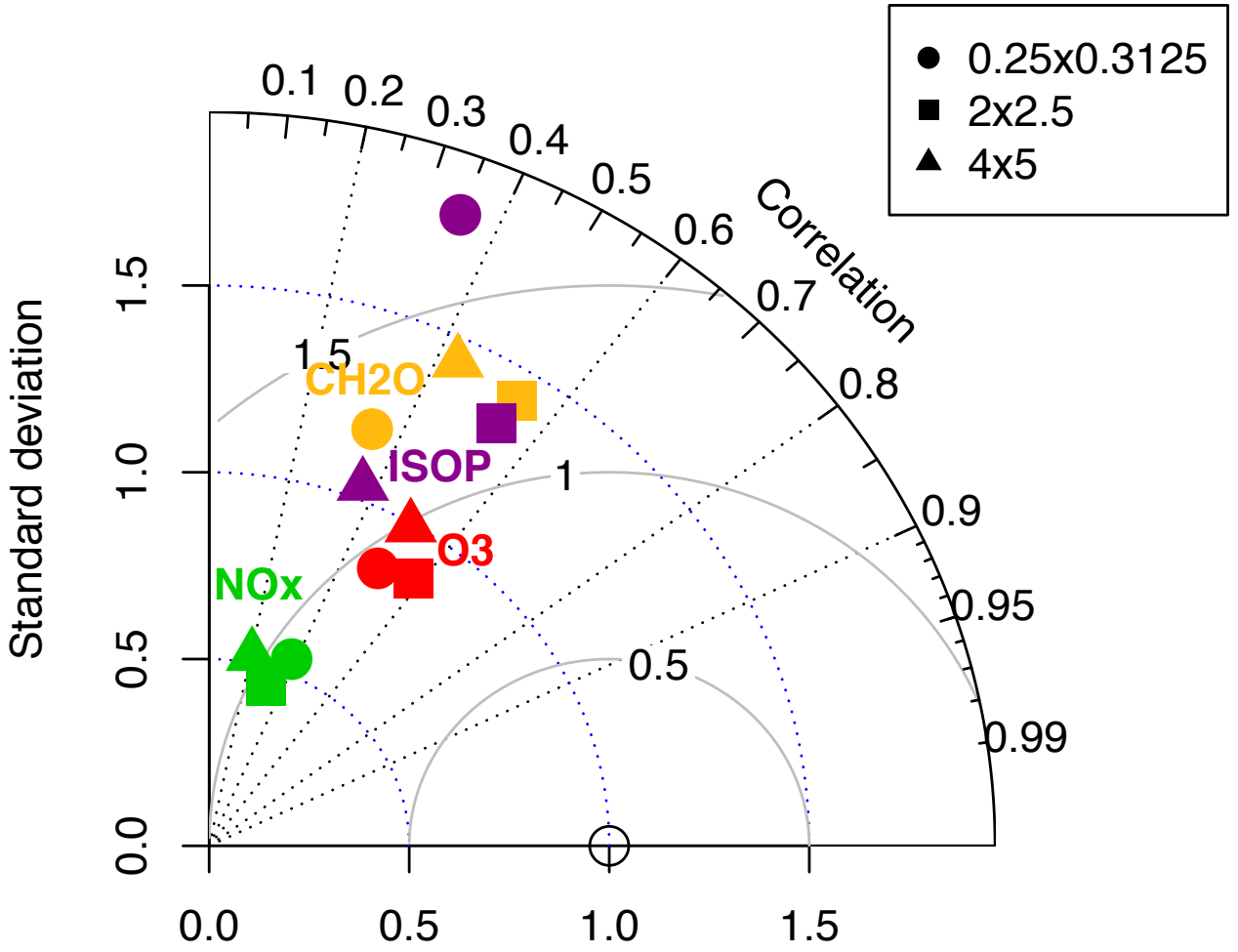


MDA8 ozone above 75 ppbv measured at AQS sites

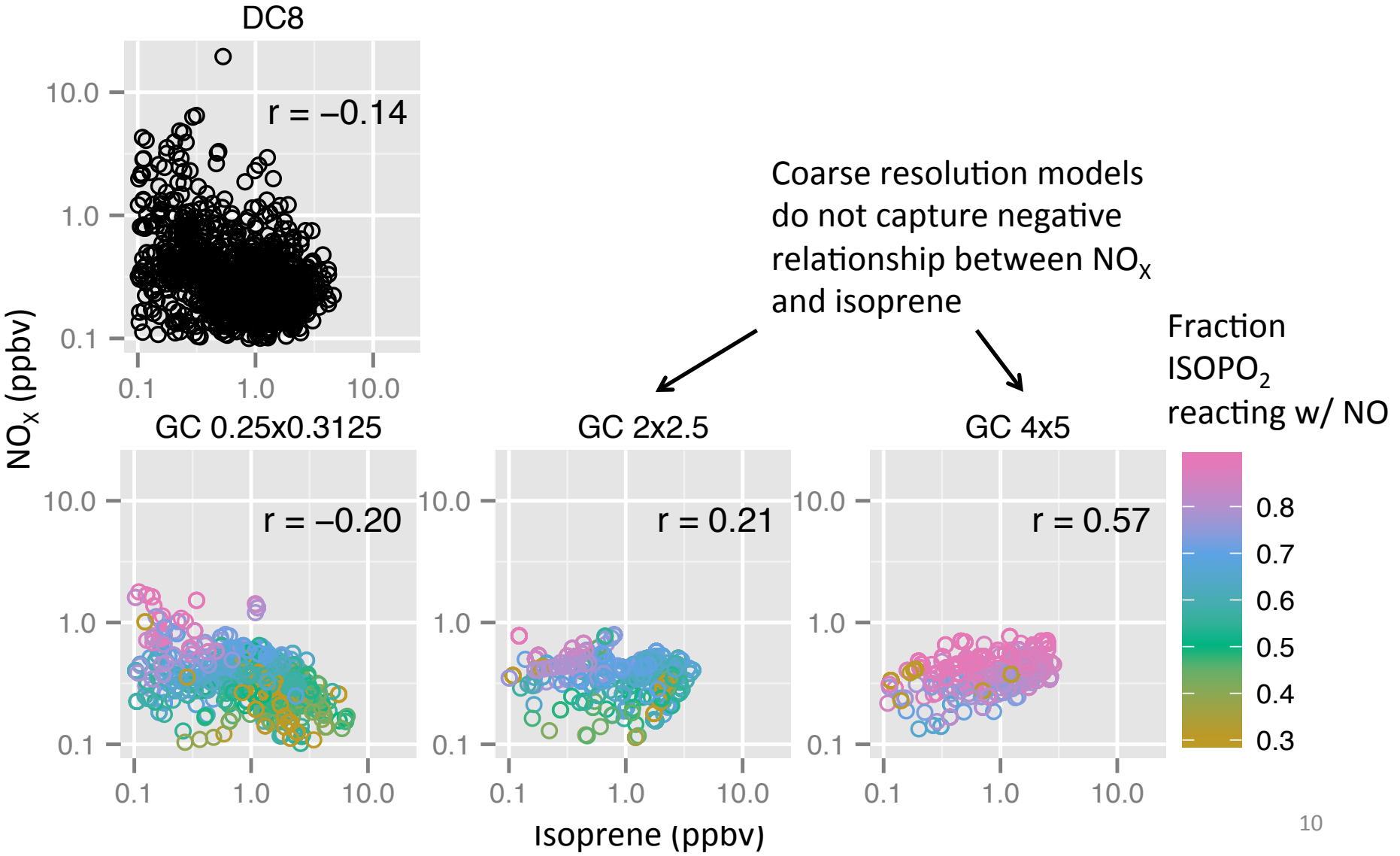


- Increasing grid resolution improves representation of high tail compared against AQS measurements.
- Measurements in the high tail are primarily urban, unlike in the SEAC^{4}RS data.

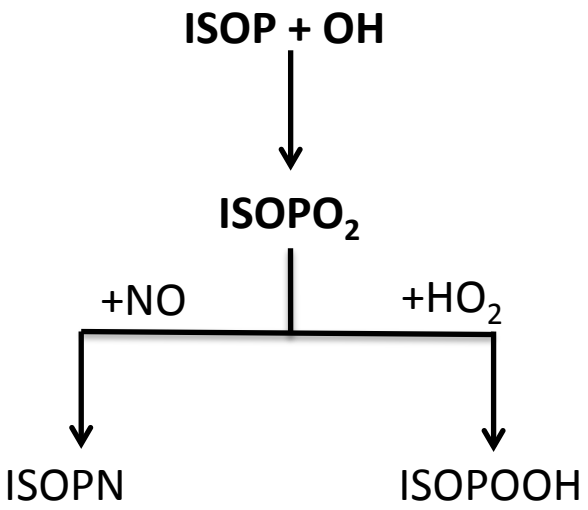
Nested model is able to capture increased variability but does not improve correlations because finer-scale variability is more difficult to capture

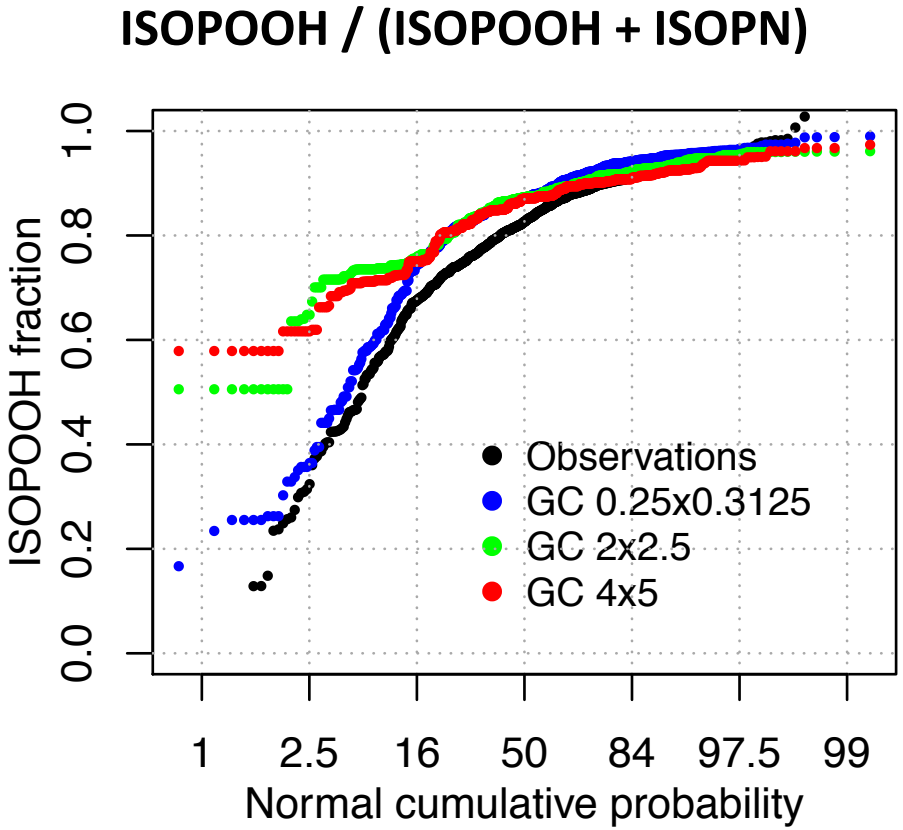


Global models are unable to distinguish high NOx from high isoprene environments, resulting in a higher fraction of peroxy radicals reacting via high-NOx pathway



SEAC^{4}RS also provides observational constraints on chemical pathways: higher resolution model improves representation of high-NOx vs. low-NOx regimes





Observations from P. Wennberg

Effect of grid resolution on regional mean concentrations is small