

# Leveraging simulated source contributions to improve understanding of atmospheric ozone

Barron H. Henderson<sup>1</sup>, Christopher Emery<sup>2</sup>, Lin Zhang<sup>3</sup>, Farhan Akhtar<sup>4</sup>, Joseph P. Pinto<sup>4</sup>

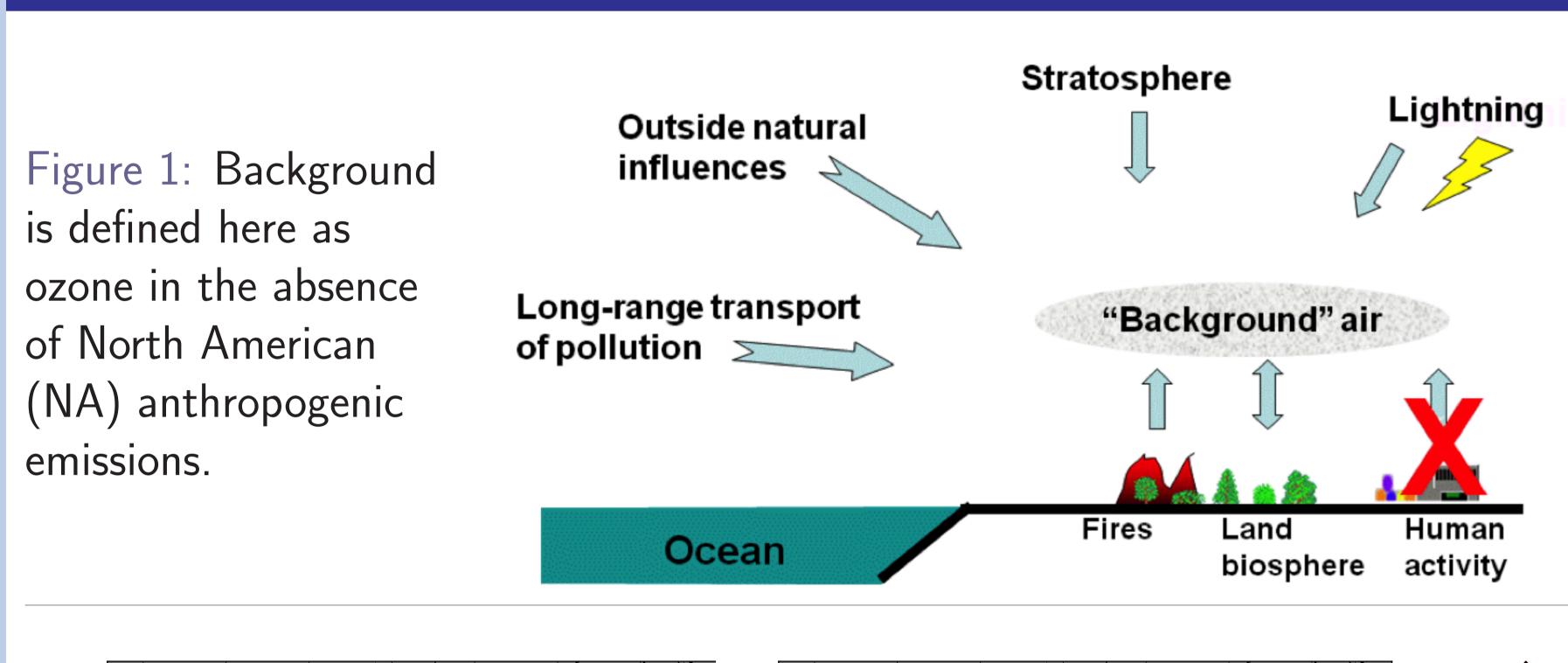


<sup>1</sup>Environmental Engineering Sciences, University of Florida; <sup>2</sup>ENVIRON International Corporation; <sup>3</sup>Peking University, Beijing, China; <sup>4</sup>Office of Research and Development, US EPA

#### Motivation

The influence of natural and intercontinental emissions on air quality has received increasing attention as 1) regulations tighten, and 2) developing nations exported pollutants increase. There is a consensus that hemispheric transport does affect ozone concentrations transported into nations including the United States of America<sup>1</sup>. Differences in simulated natural and intercontinental emissions underscore model process differences.

#### **Problem Demonstration**



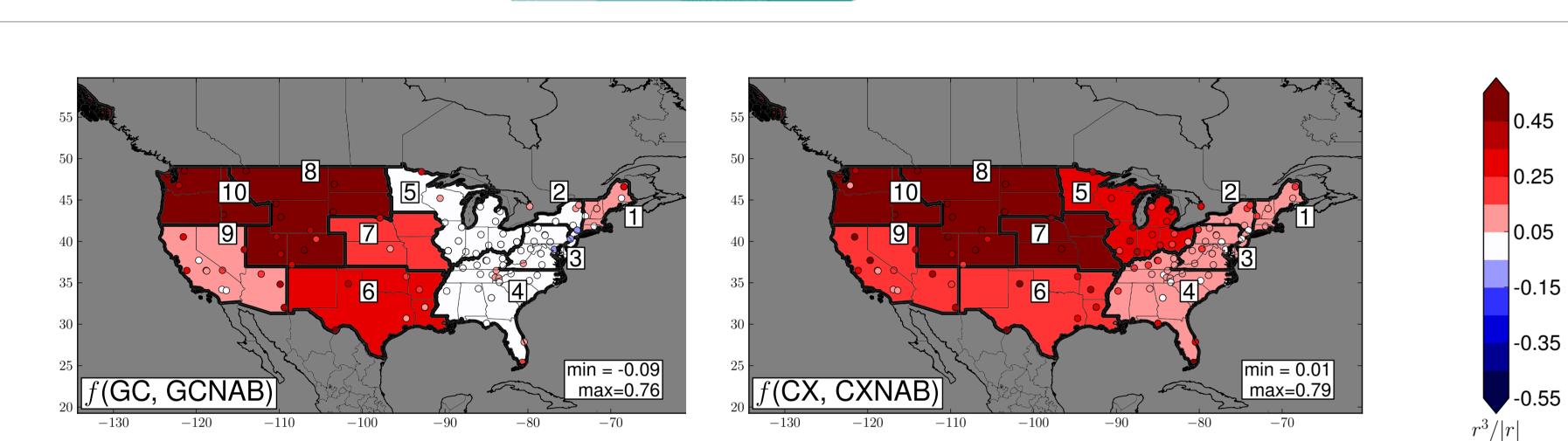


Figure 2: Signed coefficient of determination  $(r^3/|r|)$  calculated for simulations from Zhang et al.<sup>6</sup> (left) and Emery et al.<sup>2</sup> (right) demonstrate disagreement on the relationship of background and total ozone, particularly in the East.

### Modeling Results

All modeling model predictions in this analysis were developed by Zhang et al.<sup>6</sup> or Emery et al.<sup>2</sup>; key differences between the results are summarised in Table 1.

Table 1: Model configuration summary for Zhang et al.<sup>6</sup> (GC) and Emery et al.<sup>2</sup> (CX) simulations.

	GC*	CX†
Model	GEOS-Chem	CAMx
Resolution	$1/2^{\circ} \times 2/3^{\circ}$	12km x 12km
Meteorology	GEOS5	WRF
Chemistry	Version 8-02-03 <sup>‡</sup>	Carbon Bond '05§
Boundaries	GC 2x2.5°	GC 2x2.5°
Biogenic Emiss	MEGAN	BEIS
Lightning Profile	LTDIS scaled with Pick-	Scaled with Koo et al. <sup>3</sup>
	ering et al. <sup>4</sup> profile	profile
Wildfires Emiss	GFED monthly average	SmartFire daily estimate
1	. 2 *	

\*Zhang et al.<sup>6</sup>; †Emery et al.<sup>2</sup>; ‡Updates to chemistry in v8-02-04 will decrease nitrogen oxide loss to isoprene nitrates §Does not include updated isoprene as in Xie et al.<sup>5</sup>



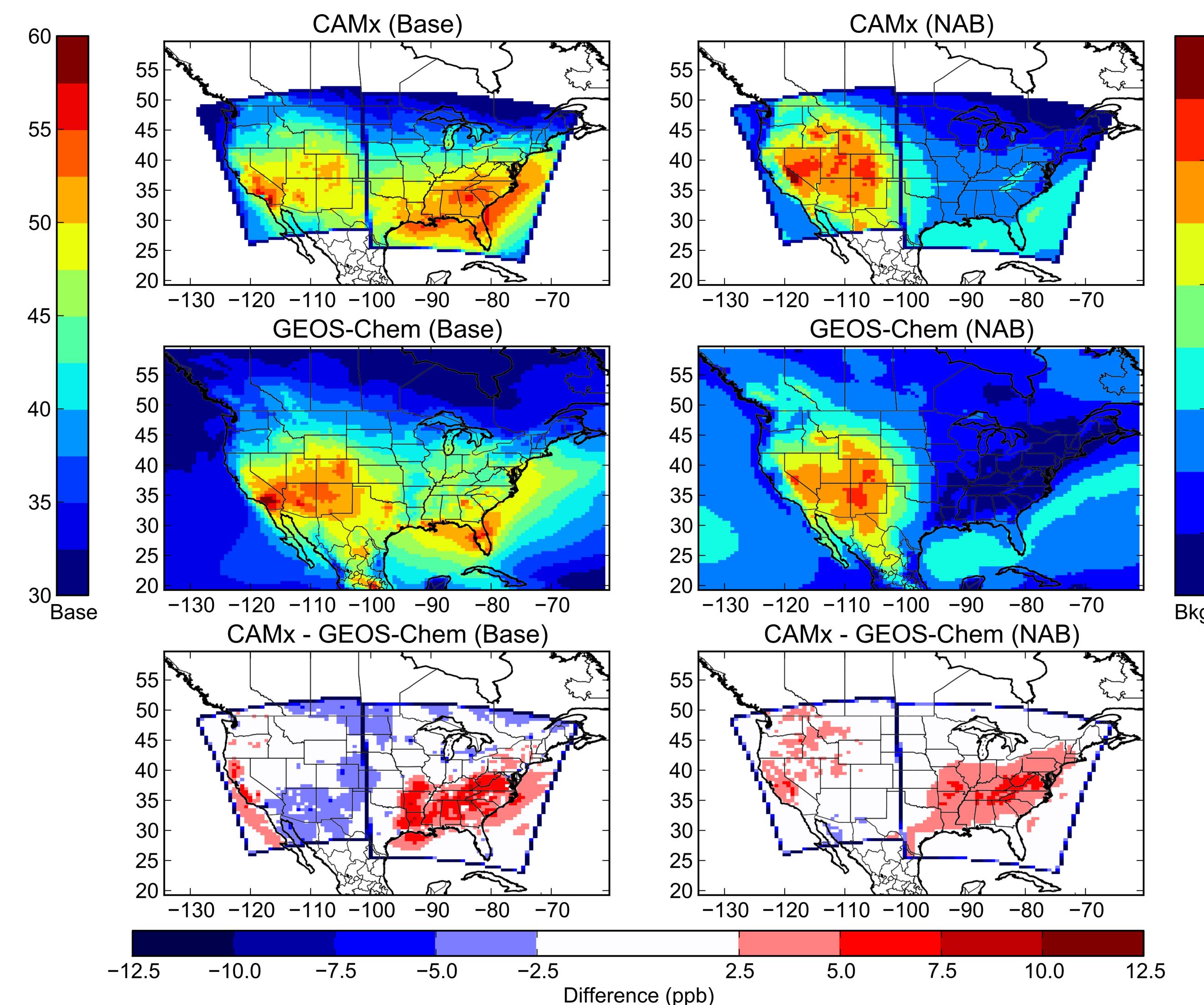
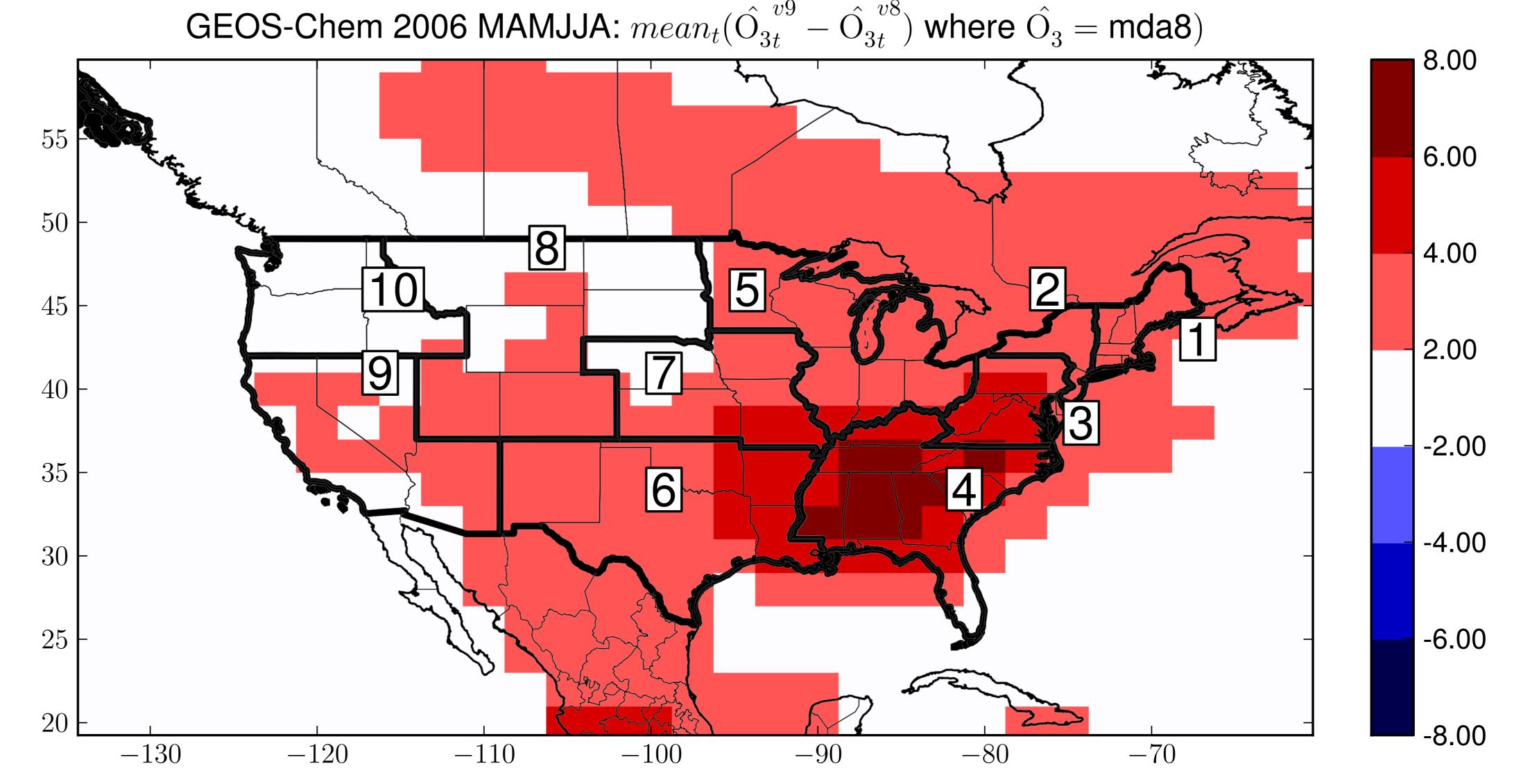


Figure 3: Maximum daily 8-hour average  $O_3$  predictions show biggest differences (based on regridding to  $1/2^{\circ}$  x  $2/3^{\circ}$ ) in the Southeast with (Base) or without NA anthropogenic emissions (NAB). NAB also shows some differences in the West.

## Isoprene Chemistry Explains Model Differences

Figure 4: Spatial distribution of average difference between of O<sub>2</sub> from GEOS-Chem with version 9 and version 8 chemistry. Version 9 chemistry reduces isoprene nitrate production in GEOS-Chem 2°x2.5° simulations, increasing ozone most in the Southeast and Mexico (not shown).



# Improving Isoprene Nitrates Increases Bias

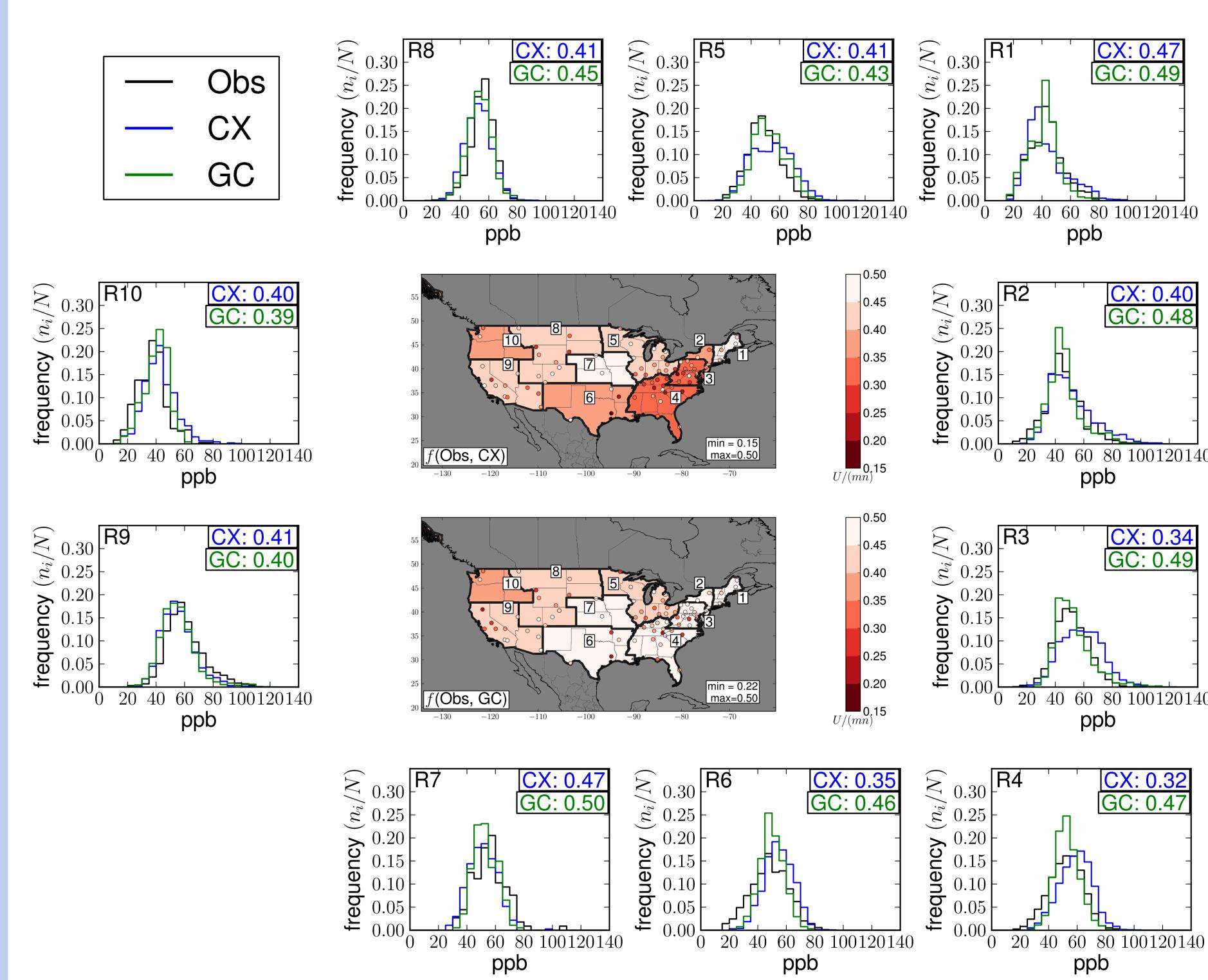


Figure 5: Mann-Whitney ho (ho=U/(mn); 0 o 0.5=worst o best agreement) score for  $O_3$  shows that reduced nitrates is associated with high-bias. CAMx/Carbon Bond '05 has lower isoprene nitrate yield – more nitrogen oxides and ozone. Similar increased bias is seen when comparing updated GEOS-Chem (not shown).

#### Summary

Background ozone, measurements and predictions, are getting increased attention because of their relevance in policy. Models inter-comparison show some inconsistent results:

- 1. largest difference between CAMx and GEOS-Chem (v8) in the East,
- 2. difference is attributable to isoprene nitrate branching ratio,
- 3. updating GEOS-Chem isoprene nitrate yield (v8  $\rightarrow$  v9) improves model consistency by increasing Base/NAB correlation and bias,
- 4. Isoprene nitrates production remains uncertain and strongly affects the NO budget, and model updates are underway<sup>5</sup>,
- 5. updated chemistry is associated with a high-bias that future chemistry updates must address.

Isoprene is a globally ubiquitous organic compound and isoprene nitrate budgets meaningfully influence NO, budgets in both present day and responses hypothetical emission reductions.

**Acknowledgments:** Supported in part by startup funds from the University of Florida and by an appointment to the Research Participation Program at EPA/NERL administered by the Oak Ridge Institute for Science and Education. Thanks also to the American Petroleum Institute for funding modeling datasets used here.

**Bibliography:** [1] Dentener et al. Hemispheric transport of air pollution. Part A: Ozone and Particulate Matter. Technical Report 17, Economic Commission For Europe, United Nations, Geneva, 2010. [2] Emery et al. Atmospheric Environment, 47:206–217, 2012. doi: 10.1016/j.atmosenv.2011.11.012. [3] Koo et al. Atmospheric Environment, 44(19): 2372–2382, 2010. doi: 10.1016/j.atmosenv.2010.02.041. [4] Pickering et al. *Journal of Geophysical Research*, 103(D23): 31203–31,216, 1998. doi: 10.1029/98 JD02651. [5] Xie et al. Atmospheric Chemistry and Physics Discussions, 12(10): 27173–27218, 2012. doi: 10.5194/acpd-12-27173-2012. [6] Zhang et al. Atmospheric Environment, 45(37):6769–6776, **2011**. doi: 10.1016/j.atmosenv.2011.07.054.